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1. REPORT DATE (DD-MM-YYYY) 30-August-2007	2. REPORT TYPE Final Technical	3. DATES COVERED (From - To) August 2006 to June 2007
4. TITLE AND SUBTITLE Aluminum Agglomeration and Trajectory in Solid Rocket Motors		5a. CONTRACT NUMBER FA9550-06-C-0069
		5b. GRANT NUMBER
		5c. PROGRAM ELEMENT NUMBER
		5d. PROJECT NUMBER
		5e. TASK NUMBER
		5f. WORK UNIT NUMBER
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Software and Engineering Associates, Inc. 1802 N. Carson Street, Suite 200 Carson City, NV 89701-1238		8. PERFORMING ORGANIZATION REPORT NUMBER SN285-Final Report
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) Air Force Office of Scientific Research 875 North Randolph Street, RM 3112 Arlington, VA 22203		10. SPONSOR/MONITOR'S ACRONYM(S)
		11. SPONSOR/MONITOR'S REPORT NUMBER(S)
12. DISTRIBUTION/AVAILABILITY STATEMENT Approved for public release; distribution unlimited.		
AFRT-SR-AR-TR-08-0139		

13. SUPPLEMENTARY NOTES

20080331066

14. ABSTRACT

Report developed un STTR contract for Topic AF06-T012. The demand for higher performance rocket motors at a reduced cost requires continuous improvements in understanding and controlling propellant combustion. Numerous examples are available where seemingly minor modifications and improvements to existing solid rocket systems have caused previously well performing motors to exhibit unexpected and at times near catastrophic behavior. It is far cheaper to design out problems than fix them during the development or production phases. Various combustion issues have never been modeled in a complete motor prediction model. What is being proposed here has never been successfully done and would greatly increase the design tools available to the motor design community.

The overall goal of this innovation is to provide a multi-physics based computer code which will accurately predict the entire flight of aluminum particles from the propellant surface through the nozzle exit plane together with a prediction of the effective properties

15. SUBJECT TERMS

Aluminum Combustion, Solid Rocket Motor, Propulsion, Modeling, Aluminum Agglomeration, Numerical Tool

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON Douglas E. Coats
a. REPORT U	b. ABSTRACT U	c. THIS PAGE U	UU	90	19b. TELEPHONE NUMBER (Include area code) 775-882-1966

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1 INTRODUCTION

1.1 Description of Document

This document is the final report on SBIR Contract FA9550-06-C-0069, "Aluminum Agglomeration and Trajectory in Solid Rocket Motors". The final report details the contractual work and effort from SEA, BYU, and ATK. The purpose of this effort was to demonstrate the feasibility of developing a software system which track Aluminum agglomerates coming off of the surface of a solid propellant and tracking them though to the nozzle exit plane in a solid propellant rocket motor. The main elements of the final report and their locations are given below.

Section 2 of our original proposal represents a good description of the state of the art in modeling aluminum combustion in solid rocket motors, SRMs, and is included as part of Appendix A. Our proposed work plan is given in Appendix B and remains a good outline of the work to be done to accomplish the overall goals of this effort. Because our two progress reports describe individual work items in greater detail than we want to discuss in the main body of this final report, they are given in Appendixes C and D. The final reports of both BYU and ATK are presented in their entirety in Appendixes E and F.

In section 1.2 of the main body of this report describes the significance and importance of the work by all three partners; it is followed by an executive summary of our efforts and results. Section 2 provides descriptions and details of the major accomplishments for each task. And, finally, Section 3 gives recommendations and conclusions for future work.

1.2 Significance of Innovation

The accurate prediction of solid rocket motor environment and performance is a recurring need during the development of new propulsion systems for the Air Force, Navy, Army and NASA. A demand for higher performance at a reduced cost requires continuous improvements in understanding and controlling both steady state and transient combustion. Numerous examples are available where seemingly minor modifications and improvements to existing solid rocket systems have caused previously well performing motors to exhibit unexpected and at times near catastrophic behavior. If motor environment and performance can be adequately characterized during the design and development process, it is far cheaper to identify and solve problems. For example, a motor technology development program that experienced a nozzle erosion failure late in the demonstration phase in CY2002 cost the prime contractor a million dollars and delayed the program more than a year. Various transient combustion issues, either intentional or not, have never been modeled in a complete motor prediction model. What is being proposed here has never been successfully done and would greatly increase the design tools available to the motor design community.

The overall goal of this innovation was to provide a multi-physics based computer code which accurately predicted the entire flight of aluminum particles from the propellant surface

through the nozzle exit plane (for nozzle impact studies and plume signature studies) together with a prediction of the effective properties (thermal conductivity and measures of mechanical strength such as Young's modulus, Poisson's ratio) of the binder, ammonium perchlorate, and aluminum particles which together constitute a solid propellant.

The crux of this innovation was a combination of appropriate physics based models incorporated into a modern software framework. The selection of the physics based models, not too simple and not too complex, was the key to producing a working model which would be able to run on computer systems becoming available in the next several years. Teraflop computing systems are available now at most large engineering firms and even some small firms such as SEA. Larger systems capable of running at hundreds of teraflops are available from government labs. The target computer system for this effort is a 10 to 100 teraflop cluster, available to the working engineer or researcher from their desktop within the next four to five years. Software requiring petaflop performance is not useful for ordinary engineering use; and hence, is not a commercially viable product.

1.3 Executive Summary

The tasks laid out for this work effort are enormous in scope as witnessed by the lack of progress made over the last decade by many smart and ingenious researchers. However, our efforts combined with those of others have been able to make good progress on defining methods to attack the problem of producing a software system which will track the process of aluminum combustion from the propellant surface to the nozzle exit and provide design guidance to rocket motor development. The original program plan for this effort consisted of five tasks which are listed below:

- Task 1. Propellant Constituent Packing Model
- Task 2. Combustion Models
- Task 3. Modeling Approaches for Droplet Size Change Mechanisms
- Task 4. Review and Select Models of Droplet Impact, Erosion, and Heat Transfer
- Task 5. Review and Select the Computer Framework Software Programs

We have made significant advances in Tasks 1, 2, and 3. In Task 4 we relied on work being performed under the AFRL sponsored IHPRT SRM Modeling and Simulation effort. Task 5 has been put off until the Phase II effort because all of the software elements were not defined in the Phase I effort.

In Task 1 we relied on the ATK developed propellant packing model, ParPack, because it contained not only a physical description of the propellant pack but also includes the prediction of the effective properties (thermal conductivity and measures of mechanical strength such as Young's modulus, Poisson's ratio) of the binder, ammonium perchlorate, and aluminum particles which together constitute a solid propellant. The question we addressed in this effort is if it is necessary to use a packing model to accurately predict the propellant burning rate. What we found is that the description of the propellant surface did not vary significantly from what would be predicted by using the average surface fraction values. Dr. Beckstead of BYU also found that

the use of the more complete chemical kinetics models was significantly more important than the surface geometry in predicting the propellant burn rate. The task for the Phase II effort is now to develop statistical methods given the mean values of AP and Al particles to feed a detailed combustion model.

Task 2 consisted of three parts, burn rate modeling, formation of Al/Al₂O₃ surface agglomerates and the ignition of the agglomerates. While no suitable models were found for the formation of Al/Al₂O₃ surface agglomerates, good progress was made by Dr. Beckstead and his students at BYU in defining an adequate kinetic mechanism to predict the propellant burning rate. The formation of Al/Al₂O₃ surface agglomerates remains a very difficult task and will be attacked in the Phase II effort.

In looking at Modeling Approaches for Droplet Size Change Mechanisms, Task 3, we discovered from running our chamber flowfield model that the collision/coalescence of Al₂O₃ smoke and agglomerates is an important mechanism in both determining alumina trajectories and in predicting how much of the aluminum is burned inside the motor. The further development of this chamber flowfield computer model will be an important part of the Phase II effort.

In task 4, Review and Select Models of Droplet Impact, Erosion, and Heat Transfer, we only selected the models necessary for the development of Task 3. Currently, we have relied on work being performed under the AFRL sponsored IHPRT SRM Modeling and Simulation effort to further define these models. We plan to review all of the IHPRT models during the Phase II effort.

Task 5 has been put off until the Phase II effort because all of the software elements were not defined in the Phase I effort.

Hence the work to be done in the Phase II effort is:

- Improve and generalize the BYU combustion model
- Improve the chamber flowfield model and include an Al agglomeration and ignition model
- Develop a multidimensional extended chamber/nozzle flowfield program
- Review and implement models of droplet impact, erosion, and heat transfer in an extended chamber/nozzle flowfield program
- Include the above models in an easy to use software framework

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2 WORK ACCOMPLISHED

The tasks laid out for this work effort are enormous in scope as witnessed by the lack of progress made over the last decade by many smart and ingenious researchers. However, our efforts combined with those of others have been able to make good progress on defining methods to attack the problem of producing a software system which will track the process of aluminum combustion from the propellant surface to the nozzle exit and provide design guidance to rocket motor development. The original program plan for this effort consisted of five tasks which are listed below:

- Task 1. Propellant Constituent Packing Model
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- Task 4. Review and Select Models of Droplet Impact, Erosion, and Heat Transfer
- Task 5. Review and Select the Computer Framework Software Programs

We have made significant advances in Tasks 1, 2, and 3. In Task 4 we relied on work being performed under the AFRL sponsored IHPRT SRM Modeling and Simulation effort. Task 5 has been put off until the Phase II effort because all of the software elements were not defined in the Phase I effort.

2.1 Accomplishment Task #1, Propellant Constituent Packing Model

In Task 1 we relied on the ATK developed propellant packing model, ParPack, because it contained not only a physical description of the propellant pack but also includes the prediction of the effective properties (thermal conductivity and measures of mechanical strength such as Young's modulus, Poisson's ratio) of the binder, ammonium perchlorate, and aluminum particles which together constitute a solid propellant. The question we addressed in this effort is if it was necessary to use a packing model to accurately predict the propellant burning rate and agglomeration of aluminum on the propellant surface.

ATK was tasked to make a propellant packing model for a typical propellant for which we had data on both the burning rate and sizes and distributions of aluminum agglomerates coming off of the propellant surface. They selected the Minuteman propellant used in the Air Force IHPRT modeling and simulation effort. The details of their work are reported in Appendix F. Figure 1 shows the distribution of total modeled AP surface area versus distance into the pack and the constant horizontal line represents the average AP surface area of 47,686 square microns with a standard deviation of 9.5%. From the propellant formulation, the average surface area was calculated as 45,045 sq. microns, a 5.86 per cent difference. We are not sure as to the exact reason for the difference; however the difference is unimportant for the purpose at hand.

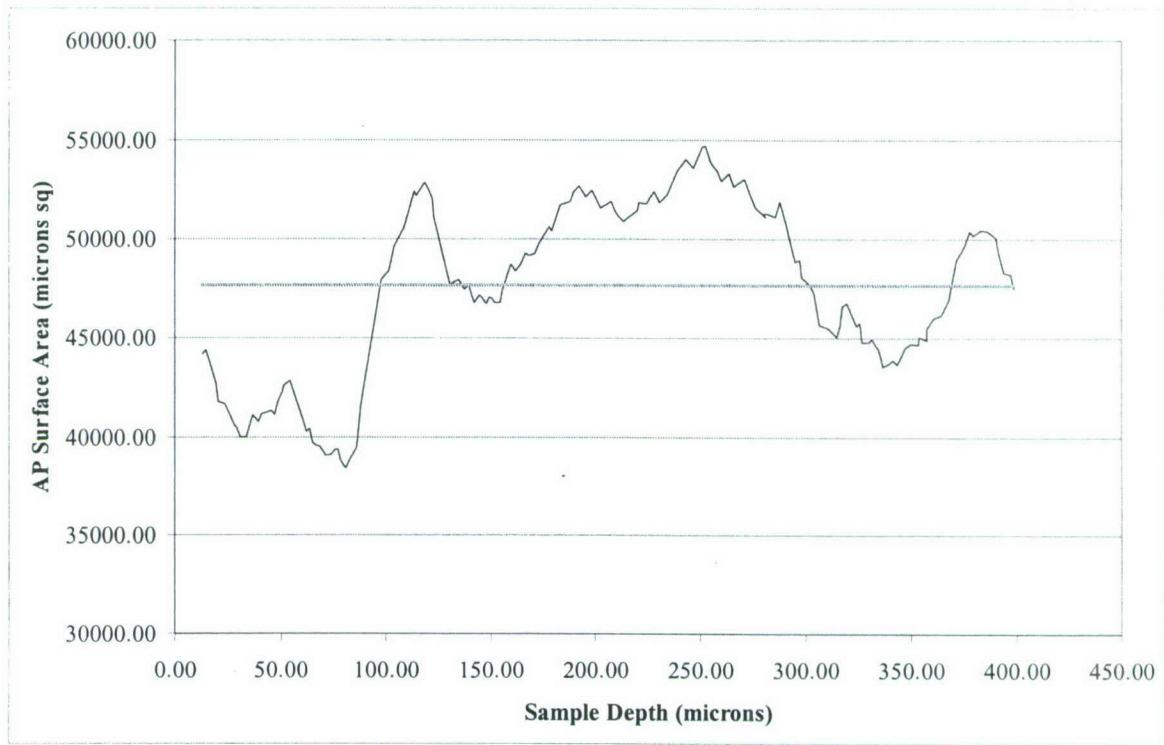


Figure 1. Exposed AP Surface Area versus Depth into the Sample Pack

What we found is that the description of the propellant surface did not vary significantly from what would be predicted by using the average surface fraction values except for the influence of the very large AP particles on our small 300 micron in diameter sample. The first conclusion that we drew from this observation is that if direct numerical simulation is to be used in either combustion model, then the size of the pack model would have to be large with respect to the large AP size. The second conclusion is that we should be able to use statistical methods around the mean sizes to represent the surface topography.

The distribution of both AP and Al particles on the surface of the propellant is important in two ways. Firstly, it has an impact on the distribution of burning AP particles and hence on the propellant burn rate. Secondly, the distribution of Aluminum particles coming to the surface is an important parameter in almost all of the agglomeration models since it indicates how many small Al particles have a chance to agglomerate together. Because the generation of a model of the propellant packing is a time consuming procedure, it is an important conclusion that either average values or a distribution function are good candidates for use in modeling both the burn rate and agglomeration sizes.

Dr. Beckstead of BYU also found that the use of the more complete chemical kinetics models was significantly more important than the surface geometry in predicting the propellant burn rate. The task for the Phase II effort is now to develop statistical methods given the mean values of AP and Al particles to feed a detailed combustion model.

2.2 Accomplishment Task #2, Combustion Models

Task 2 consisted of three parts, burn rate modeling, formation of Al/Al₂O₃ surface agglomerates, and the ignition and burning of the agglomerates coming off the surface of the propellant.

Dr. Beckstead and his students at BYU have made good progress in defining an adequate kinetic mechanism to predict the propellant burning rate, see Appendix E. As mentioned above, the use of a more complete chemical kinetics models was found to be significantly more important than the surface geometry in predicting the propellant burn rate.

In addition to the burn back of the propellant surface, the size distribution and subsequent combustion of the aluminum/Al₂O₃ agglomerates leaving the surface of the propellant is a fundamental boundary condition required for simulating the solid rocket motor environment and performance. The modeling of aluminum combustion in a SRM along with predicting the trajectory of the burning aluminum/alumina droplet within the motor depends on many factors. Chief among these factors is the knowledge of the size and composition of the burning aluminum agglomerates coming off of the surface of the propellant. Also required are the rate at which these agglomerates burn, and any collision/coalescence and breakup of the droplets within the motor.

The formation of Al/Al₂O₃ surface agglomerates remains a very difficult task and will be further addressed in the Phase II effort. In the meantime, we will use existing models and correlations for the agglomeration process. The correlations due to Dr. Robert Hermsen in the SPP code¹ and Liu² will be used along with the Cohen's³ Pocket model to predict agglomerate sizes when data are not available.

Of the modern analytic models of agglomeration which are usually referred to as "pocket models", the model due to Srinivas and Chakravarthy⁴ is the most appealing. This model includes a random seed packing model to keep track of the rate at which the aluminum is coming to the surface and establishes the residence time on the propellant surface by using a kinetically limited AP leading-edge flame as the aluminum ignition mechanism. As part of the Phase II effort, we would replace the packing model with a statistical equivalent model.

The uncertainty in the agglomerate size precludes the use of a sophisticated model for the burn rate of the aluminum droplets and agglomerates. For our baseline use we have selected the empirical models of Dr. Hermsen⁵ and Dr. Beckstead⁶. Both of these models are of the simple

¹ Nickerson, G. R., Coats, D. E., Dang, A. L., Dunn, S. S., Hermsen, R. W., "The Solid Propellant Rocket Motor Performance Computer Program (SPP), Version 6.0", Vol. I, AFRPL TR-87-078, December 1987.

² Liu, T-K., "Experimental and Model Study of Agglomeration of Burning Aluminized Propellants," *Journal of Propulsion and Power*, vol. 21, no. 5, Sep.-Oct. 2005, pp. 797-806.

³ Cohen, N.S., "A Pocket Model for Aluminum Agglomeration in Composite Propellants," AIAA-81-1585, 17th AIAA/SAE/ASME Joint Propulsion Conference, Colorado Springs, CO, July 27-29, 1981.

⁴ Srinivas, V., Chakravarthy, S.R., "Computer Model of Aluminum Agglomeration on the Burning Surface of a Composite Solid Propellant," AIAA 2005-743, 43rd AIAA Aerospace Sciences Meeting & Exhibit, Reno, NV, 2005.

⁵ Hermsen, R. W., "Aluminum Combustion Efficiency in Solid Rocket Motors," AIAA-81-0038, AIAA 19th Aerospace Sciences Meeting, St. Louis, MO, January 12-15, 1981.

D^2 type. The two models are similar, differing in only the oxidizing species considered and some constants. Both models take the form:

$$\frac{d(m_{Al})}{dt} = -\frac{\pi}{2} \rho_{Al} \frac{k}{1.8} D_p^3 D_p^{-1.8} \quad (1)$$

The open question in using such models is the fraction of alumina which is left on the droplet as an oxide cap.

2.3 Accomplishment Task #3, Modeling Approaches for Droplet Size Change Mechanisms

The major size change mechanisms, other than burning, are collision/coalescence of smaller droplets with larger ones and droplet breakup. We developed a prototype chamber flowfield code assuming quasi one dimensional flow with collision/coalescence, droplet burning, and droplet breakup. The collision/coalescence model was that recommended by Salita⁷, the burn rate model was that of either Hermesen or Beckstead, and the breakup model was based on a Weber number criterion.

During our investigation of Modeling Approaches for Droplet Size Change Mechanisms, Task 3, we discovered from running our chamber flowfield model that the collision/coalescence of Al_2O_3 smoke and agglomerates is an important mechanism in both determining alumina trajectories and in predicting how much of the aluminum is buried inside the motor. In fact, for long length to diameter motors, it is a dominant mechanism in determining the size of the droplet entering the nozzle. The further development of this chamber flowfield computer model will be an important part of the Phase II effort.

2.4 Accomplishment Task #4, Review and Select Models of Droplet Impact, Erosion, and Heat Transfer

In Task 4, Review and Select Models of Droplet Impact, Erosion, and Heat Transfer, we only selected the models necessary for the development of Task 3. Currently, we have relied on work being performed under the AFRL sponsored IHPRT SRM Modeling and Simulation effort to further define these models. We plan to review all of the IHPRT models during the Phase II effort.

Of particular interest is the HERO2D⁸ particle impact and erosion model developed by ATK/Thiokol under the IHPRT program. The code has not been officially released as of yet

⁶ Beckstead, M. W., Newbold, B.R., and Waroquet, C., "A Summary of Aluminum Combustion," 37th JANNAF Combustion Meeting, CPIA No. 701, Vol. 1, November 2000, pp. 485-504.

⁷ Salita, M., "Simulation of Al_2O_3 Collision/Coalescence Using Water and Mercury Droplets", Thiokol TWR-40224, 5/18/89; also 26th JANNAF Combustion Meeting (JPL), 10/89.

⁸ M. E. Ewing, D. T. Walker and D. A. Isaac. "Development of a two-dimensional numerical code for modeling pyrolysis and ablation". *JANNAF 54th JPM, 3rd LPS, 2nd SPS, and 5th MSS Joint Meeting*, Denver, CO, 14-17 May 2007

and we plan to evaluate it once it becomes available. SEA's own effort, see Appendix D, has been in automating a classical diffusion limited thermochemical erosion model.

2.5 Accomplishment Task #5, Review and Select the Computer Framework Software Programs

Implementation of Task 5 has been put off until the Phase II effort because all of the software elements were not defined in the Phase I effort. However, SEA has been investigating various methods of implementing a cross platform Graphical User Interface for tying the various computation models together in a unified fashion.

Initially, SEA's SPP code and ATK/Thiokol's FEM-BUILDER code were considered as candidate frameworks for the aluminum combustion and flow solver models. Concurrent work performed by SEA as part of the IHPRT program has produced a Perl⁹-based driver script for SPP and other codes. This script calls each module as an individual executable. Communications between modules will be coordinated by this script through various data files. At present, this script exists only in command line mode, though a graphical interface is being developed for SEA's TDK code.

Positioning a high-level driver script on top of SPP and/or FEM-BUILDER and other codes appears to offer a very general and flexible framework. Such a framework is likely to facilitate the integration and inter-operation of aluminum-combustion and flow-solution modules within the code to be developed in the Phase II effort and other codes. It also facilitates the development and perhaps even the automatic configuration of a graphical user interface via the GTK+ toolkit and gtk2-perl¹⁰.

Perl is a stable, cross-platform programming language. It is very well-suited to manipulating text-based files, such as the input and output files used by the Phase II code. This makes it an ideal scripting language for the task at hand. GTK+¹¹ is a multi-platform toolkit for creating graphical user interfaces. It is free software, developed as part of the GNU Project. It is licensed under the GNU LGPL, which allows it to be used by all developers, including those developing proprietary software, without any license fees or royalties. Gtk2-perl is the collective name for a set of Perl bindings for GTK+ and various related libraries. These modules make it easy to write graphical applications using Perl.

⁹ The Perl directory. <http://www.perl.org/>, 2007.

¹⁰ Gtk2-perl. <http://gtk2-perl.sourceforge.net/>, 2007.

¹¹ GTK+ — The GIMP toolkit. <http://www.gtk.org/>, 2007.

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3 RECOMMENDATIONS AND CONCLUSIONS

One of the many problems associated with a design tool is the time and effort required to evaluate the effect of a design change. In many cases, answers are needed in minutes while others can wait hours or overnight. Seldom will designers wait for days or weeks for an answer to any but the most important questions. On the other hand, once the motor or prototype is built, the time scales in answering questions changes. In other words, there is a non trivial hierarchy in the design process with certain elements requiring different time scales for solutions at different times in the development of the motor. Any code which purports to be general design tool for developing solid rocket motor's, SRM's, must take these factors into account or it will not be used.

In their 2008 AIAA paper, Buckmaster and Jackson¹², discussed a number of the problems associated with designing a SRM.. Unfortunately, they only alluded to solutions to some of the problems. Modeling the combustion processes in a SRM is a daunting challenge, but modeling the motor throughout its entire burn time is even more so. A design tool to be complete must model not only the propellant properties, but also handle the entire burn time from ignition to burn out taking into account the thermal and structural factors along with the performance of the motor. In our Phase I effort, we have investigated only some of the areas needed to completely model a SRM, and what we proposed for the Phase II effort is still only a subset of the total problem, though more complete than discussed by Buckmaster et al.

SEA's SPP code treats the performance of a SRM from ignition to tail off. It models the burning and shape change of the solid propellant, erosion of the nozzle, incomplete combustion of the metal in the fuel, and accounts for finite rate chemistry and two phase flow losses in the nozzle as well as boundary layer losses. It also has a module for evaluating the potential for combustion instability. However, the code is far from complete in that many of the effects it treats are done so with simple models or empiricisms. The various types of models are listed in Table 1 below along with the application to which the model belongs. Areas for improvements to the existing SPP models or a SRM design toolkit and additions of new models are discussed in the following sub-sections.

¹² Buckmaster, J., and Jackson, T., "Developing Design Tools for Solid Propellant Rockets", AIAA-2008-0936, Aerospace Sciences Meeting, Reno, NV, Jan. 2008.

Table 1. Models to Improve Existing SPP

Type of Model	Application
Packing Model	Propellant Properties
Detailed Surface Kinetics & Diffusion	Propellant burn Rate and Agglomeration
Surface Agglomeration Model	Combustion Efficiency, Slag, & Erosion
Collision/Coalescence Model	Combustion Efficiency, Slag, & Erosion
Droplet Breakup Model	Nozzle Performance Loss
Surface Morphological Model	Propellant Burn Rate and Agglomeration
Chamber Flowfield Model	Metal Combustion and Collision/Coalescence Particle Impact, Erosion, & Slag Accumulation
Grain Design and Ballistics And Ignition and Blow Down Transient	Thrust Time History Beginning & Ending Thrust-Pressure Trace
Combustion Stability Models	Evaluate Potential for Unstable Operation
Heat Transfer and Erosion Model	Determine Design Margins for the TPS

Packing Models

The existing ATK ParPack model has been demonstrated to accurately predict propellant physical properties. The utility of packing models in predicting propellant burn rates and metal surface agglomeration have yet to be demonstrated. To date the packing codes have only been able to predict the correct answer for burn rate and agglomerate once the answer is known. Improvements to the packing model proposed by Buckmaster et al.¹³ ignore the fact that the propellants as poured in a motor are not isotropic or homogeneous, nor are the particles, AP and Al, spherical in nature. A statistical description of the propellant surface is more likely to be of practical use than a packing model for burn rate and agglomeration prediction.

Detailed Surface Kinetics & Diffusion Models

The BYU combustion model has shown that the effects of realistic detailed finite rate kinetics are more important than surface morphological effects. Hence we believe that there is a greater payoff in improving and generalizing the BYU combustion model than in further effort with the packing model.

Surface Agglomeration Model

While the size and distribution of the metal agglomerates coming off of the surface of the propellant is a fundamental boundary condition for chamber flowfield models, the sensitivity of

¹³ Op cit

the overall solution to this quantity has not been established. Considering the difficulty in formulating a physical model of the process, we should try to establish how accurately we need to know the answer before we embark on this elusive quest. To establish the required accuracy needed for the agglomeration model, we must include the effects of collision/coalescence, droplet burning rate including oxidizer depletion, and droplet breakup. Once we have these models in place, we can try to establish the sensitivity of agglomerate size on combustion efficiency, slag accumulation, droplet impact and erosion, and nozzle performance by parametrically varying this parameter.

The above recommendation does not mean that we should completely abandon modeling efforts in this area. Instead, we should limit our efforts to building the tools required for a physically based agglomeration model. From what we understand of the process, the smallest Al particles come to the surface, migrate through the melt layer and are carried away with the flow. These very small particles are then melted, ignited, and burned in the flame zone just off of the propellant surface. The largest particles, 50 microns and above, come to the surface, are heated up but at best only partially melted before the propellant burns out underneath them and they are carried away by the propellant gases. It is between these two sizes that agglomeration occurs; particles in close proximity to each other melt or become sticky and agglomerate to each other. From photographic observation, these mid size particles keep on agglomerating until they ignite at which point they leave the surface. Various models have tried to figure out the number of particles which can agglomerate and how long it would take them to ignite and thus leave the surface. The model of Srinivas and Chakravarthy seems to be the most promising and it assumes that the particles keep agglomerating until they intersect the diffusion flame of the larger AP crystals at which point they ignite. Thus we have a model which requires two characteristics of the propellant surface distribution. Since both the distribution of AP and Al can be described by multimodal log normal distributions, then the two factors driving this model should be determinable by statistical means, either closed form or by Monte Carlo simulation, thus bypassing the need for direct numerical simulation as is done in a packing model.

Collision/Coalescence Model

For the time being, the recommendation of Salita for collision/coalescence modeling is considered adequate. The large number of unknowns indicates that our resources can better be spent elsewhere. However, the literature should be searched for more appropriate models.

Droplet Breakup Model

There are a number of droplet breakup models which can be tried in order to determine the sensitivity of the model inputs to the predicted resultant droplet size. Since trying these models would require a modest effort, it is recommended that we do this task.

Surface Morphological Model

Both surface agglomeration and propellant burn rate require some information about the surface morphology. We feel that the statistical approach outlined in the surface agglomeration discussion offers the largest payoff for the effort.

Chamber Flowfield Model

There are many levels of chamber flowfield modeling, from simple 1-D quasi steady up to full 3-D Navier-Stokes with large eddy simulation codes. All of these models have their place in a palette of motor design tools. However, for the Phase II effort with limited funds, we feel that the emphasis should be on the simpler tools. Integrating a 3-D Navier-Stokes code into a design tool kit could easily consume all of the resources available. Hence we feel that the greatest payoff is for continued development of a time accurate quasi 1-D code linked to the 3-D grain design code within the SPP. The code should be fully two-phase flow with reacting chemistry, contain particle combustion models, treat collision/coalescence, and particle breakup. In addition, the code should be capable of linking to the multi-dimensional nozzle flow field solvers at user specified time intervals and also compute heat transfer coefficients for insulation and nozzle erosion studies.

The need for multidimensional chamber flow can be treated by SEA's IMPRESS 3-D flow solver which is already linked to SPP's 3-D grain design module.

Grain Design and Ballistics

and

Ignition and blow down transient

These two topics have been lumped together since they have many of the same requirements. Currently, the SPP code has two quasi-steady interior ballistics modules and an ignition transient module. The addition of the 1-D time accurate two phase flow chamber flow field module will meet most of the requirements of a motor designer. The only major addition will be the inclusion of a nozzle thrust termination option. This option should include blow out ports and propellant burn out and re-ignition. Note that the 1-D chamber flowfield model/combustion efficiency model is an integral part of this recommendation.

Combustion Stability Models

Neither the AFRL IHPPT M&S effort or Buckmaster et al.'s paper mentioned the problems associated with combustion stability even though stability problems have caused as many difficulties as most of the other area's combined. SEA has in its SPP code an integrated 1-D linear combustion stability module and stand alone versions of a 3-D code and a non-linear code. The latter two codes should be integrated into the overall SRM design toolkit software system.

Heat Transfer and Erosion Model

As part of the AFRL IHPPT M&S effort, SEA is integrating a classic 1-D diffusion limited thermochemical erosion and heat transfer module. Also as part of the same effort, ATK is developing a 2-D model which includes the effects of Al/Al₂O₃ impingement and melt

layer¹⁴. Both of these models should be included into the overall SRM design toolkit software system.

Final Conclusion and Recommendation

We believe that the Phase I effort has demonstrated the feasibility of developing a software system capable of tracking aluminum agglomerates from the propellant surface to the nozzle exit plane of a SRM. Furthermore, we have identified a number of very important phenomena which need to be modeled in order to accomplish this task, the most important of which is collision/coalescence of droplets and smoke in the chamber flowfield. We have also come to the conclusion that a direct numerical simulation propellant packing model is not required for the combustion and fluid flow models thus greatly simplifying the software system and reducing the compute times. Table 2 summarizes the models that should be included in the Phase II effort.

Hence, we recommend that a Phase II effort be funded to develop a SRM software design toolkit to not only track the burning aluminum which was the focus of this effort, but to aid in answering a large number of motor design questions. The basis for this system will have its roots in SEA's SPP code while the shell into which it would fit would be an existing framework program or a newly developed code. ATK's FemBuilder is an existing framework program and there are also a number of commercial codes available.

Table 2. Summary of Models to be Included in Phase II Effort

Recommendation	Phase II Effort
Packing Model	Not Required for combustion modeling, include for physical properties
Surface Agglomeration Model	Limit until results sensitivity to agglomerate size are known
Collision/Coalescence Model	Include
Droplet Breakup Model	Include
Chamber Flowfield Model	Include
Grain Design and Ballistics & And Ignition and blow Down Transient	Include 1-D Chamber Flowfield Model/Combustion Efficiency Model
Combustion Stability Model	Include
Heat Transfer and Erosion Model	Include

¹⁴ M. E. Ewing, D. T. Walker and D. A. Isaac. "Development of a two-dimensional numerical code for modeling pyrolysis and ablation". *JANNAF 54th JPM, 3rd LPS, 2nd SPS, and 5th MSS Joint Meeting*, Denver, CO, 14-17 May 2007

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APPENDIX A: PHASE I TECHNICAL OBJECTIVES

To accomplish the overall goal of the contract required the successful completion of the following specific objectives:

1. Develop a propellant constituent packing model capable of prediction of the particulate distribution and effective material properties.
2. Select and/or develop a suite of combustion models for predicting
 - A. The burning back of the propellant surface.
 - B. The formation of aluminum/Al₂O₃ surface agglomerates, including the aluminum and aluminum/Al₂O₃ droplet size distribution.
 - C. The ignition and burning of the aluminum/Al₂O₃ agglomerate droplets.
3. Review and select multi-dimensional, multiphase computational fluid dynamics (CFD) modeling approaches that can be used to incorporate the combustion models along with appropriate droplet coalescence/breakup models and droplet ballistic trajectory models.
4. Review and select models of droplet impact, erosion, and heat transfer on motor components, such as the internal insulation and nozzle.
5. Review and select the computer framework software programs in which the physical models will be implemented.

Each of the above specific objectives is reviewed in terms of the current State of the Art (SOTA) and the questions answered to determine the feasibility of the proposed approach.

A.1 Propellant Constituent Packing

Particle packing algorithms are essential to physics-based models of solid rocket propellant behavior. These algorithms provide the particulate distribution and material properties required as input for combustion and related motor environment models. We have made substantial progress in the areas shown in Figure A-1. The most developed of these, the micromechanical model, is nearing completion and has made accurate predictions.

We have assembled a team that has the necessary expertise in each critical area to enhance the state of the art in propellant combustion and aluminum agglomeration predictions. The beginning point for this effort is the propellant particle pack.¹

¹ Lee Davis, "Particle Pack Influence on Highly Filled Material Properties", Current Opinion in Solid State and Materials Science 4, Pergamon Press, 505, 1999.

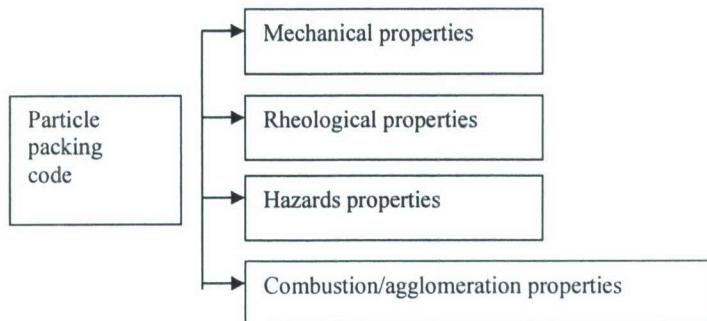


Figure A-1. Particle packing is critical to the development of material behavior models and has been used in the development of mechanical, rheological, and hazards analysis. This proposal will focus on combustion and aluminum agglomeration.

The SEA/BYU/ATK team is in the best position to advance the state of the art during this program because they (1) have the critical skills, (2) possess state of the art models & data, and (3) have the greatest amount of real-life experience and lessons learned in each area.

Many particle packing algorithms exist. Experience has dictated we use great caution in the selection of packing algorithm for the following reason. Most material properties (e.g., mechanical, rheological, ballistic, thermal, dielectric) with low to moderate particle volume fraction are insensitive to the details of the packing algorithm as long as the particle volume fraction is correct. However, for highly filled particulate materials such as solid rocket propellants, the sensitivity to packing algorithm details becomes profound. The reason for this is that the particles are so close together that small algorithmic changes can change the distribution of surface-to-surface distances on which properties so strongly depend.

Choice of packing algorithm is critical for accurate descriptions of many propellant properties.

Almost two decades have now been spent formulating, modifying, and refining a packing algorithm that more closely reflects the nature of propellant particle packs. Those efforts have resulted in a packing code called PARPACK used in all material models which depend on pack microgeometry. PARPACK is built to specifically address issues critical to propellant properties.³

- **Broad particle size distributions**
Propellant particles range from a few microns to a few hundred microns in size. PARPACK is unique among all particle packing codes in its ability to span the entire range of propellant particle sizes.
- **Particle surfaces are nearly touching but do not touch**

³ I. Lee Davis, Roger G. Carter, "Random Particle Packing by Reduced Dimension Algorithms", *Journal of Applied Physics* 67(2), 1022, Jan 1990.

The final simulated particle pack must not allow particles to contact each other. Propellant particles that touch can not be processed. Subsequently, if the particles touch there would be disastrous mechanical properties.

- **Mean surface-to-surface distance distributions**

Surface-to-surface distances average roughly two orders of magnitude smaller than the particle diameters for most propellants. As an example, the microstructurally calculated propellant shear modulus increases by almost a factor of two if the surface-to-surface distribution is used rather than just the mean surface-to-surface distance. The higher modulus matches propellant data. The packing code must reflect the microgeometry of the propellant rather than just assemble a random particle pack.

PARPACK is unique among particle packing codes. It more accurately reflects actual propellant pack microgeometry on which many propellant properties critically depend.

Table A-1 compares and contrasts classes of packing algorithms and states their pros and cons. Our recommendation, PARPACK, is highlighted in the table where it is listed as a reduced-dimension, ballistic-deposition algorithm. It therefore naturally packs small particles into the interstitial spaces of larger particles. That ability is important in the concept of pocketing which some (but not all) propellants exhibit, depending on their pack morphology. Pocketing, for those propellants that exhibit it, is crucial in aluminum agglomeration predictions.⁴

Table A-1. Particle Packing Algorithms and Their Fidelity to Real Pack Microgeometries

Highlighted packing algorithms provide the unique capability required by this program.

NAME	DESCRIPTION	PROS	CONS
Molecular dynamics	Let particles move under influence of neighboring potentials until they find close pack state	Should give realistic packs	Extremely computationally intensive; unmanageably so for broad size distributions
Random seed	Randomly spray center positions of particles in volume and let them expand until they overlap; limited movement allowed when overlaps begin	Computationally fast. Can treat moderate particle size distributions (spanning 1 order of magnitude)	Particles sprayed in by random number generator cannot mimic micro-geometry of natural packs
Random seed with dynamics (Labachevsky-Stillinger)	Randomly spray center positions, let them grow to appropriate size while dynamics is moving them to find best pack	Very dense packs that should mimic natural pack microgeometry	Extremely computationally intensive; unmanageably so for broad size distributions
Ballistic	Drop or otherwise release	Computationally	Does not create as dense

⁴ I. Lee Davis, "The Effect of Propellant Variables on Slag in Subscale Spin Motors, Part III of III, Microstructural Basis for Experimental Results", 1995 JANNAF Propulsion and Subcommittee Joint Meeting, MacDill AFB, Tampa, Florida, 1995.

deposition	particles that gravitate toward pack center as closely as possible, rolling on already-placed particles	fast unless treating broad size distributions; then computationally unmanageable	packs as molecular dynamics by a few percent
Reduced-dimension ballistic deposition (PARPACK)	Uses ballistic deposition with reduced dimension algorithms, which are phantom packs of fine particles whose statistics are based on limited packs of real fines	Computationally fastest of all routines. Unique in its ability to treat realistic packs with broad size distributions	Does not create as dense packs as molecular dynamics by a few percent
Reduced-dimension molecular dynamics (not coded yet)	Creates reduced-dimension packs and then finds closer pack conformations via molecular dynamics within reduced-dimension constraints	Should give realistic packs with broad size distributions at higher volume fraction	Will be computationally intensive but manageable so even for broad size distributions

Any of these packing algorithms can be trivially extended to create spheroidal particles, and in fact, to create ellipsoidal particles. However, years of ballistic data show that combustion is insensitive to aluminum shape. Figure A-2 shows typical aluminum used in solid propellants. It is quite irregular and generally not well described by spheroids.

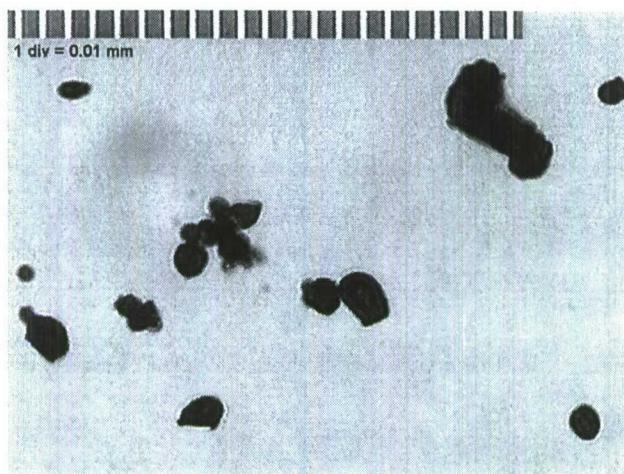


Figure A-2. Photomicrograph of Typical Aluminum Used in Solid Rocket Propellants

A.2 Combustion Models

A suite of three models is required to characterize the primary combustion mechanisms of interest related to solid rocket motor environments and performance.

A.2.1 Burn Back of the Propellant Surface

One of the desirable characteristics of AP composite propellants is the dependence of their burning rates on the size distribution of particles used. Various burning rate models have been developed over the years in an attempt to predict the effects of changing propellant formulation and operating conditions on the complex combustion of composite propellants. An early 1-D model that enjoyed some success in modeling the combustion of composite propellants was that of Beckstead, Derr and Price (BDP).^{5,6} Their 1-D model considered three separate flame zones and treated their interaction with simple global kinetics while describing the surface decomposition via pyrolysis relations. Calculations were in agreement (~10-15%) with the experimentally-observed burning rate and pressure exponent, as well as the effects of particle size and oxidizer concentration on burning rate.

Since then, these types of models have progressed through various levels of complexity, from 1-D to multi-dimensional models, and from global or semi-global gas phase kinetics to detailed reaction mechanisms with tens of species and hundreds of reactions.

Tremendous progress has been achieved in the last ten years with respect to the various modeling approaches to describe solid propellant combustion. The vastly increased performance of computing capabilities has allowed calculation schemes that were previously only conceptual.

Four areas of recent activity and interest are: first, numerical modeling of premixed flames using detailed kinetic mechanisms; second, development of packing models to calculate a geometrical distribution of particles simulating a heterogeneous solid propellant; third, coupling the packing code with a calculation of the AP/hydrocarbon diffusion flame effects to predict the burning rate of solid propellants; and fourth, applying the packing codes to attempt to predict aluminum agglomeration potential in solid propellants.

In the first area, recent modeling work using detailed kinetic mechanisms has been evolving and successfully applied to solid propellant ingredients based on a one-dimensional approach (e.g. see references^{7,8,9}). The approach allows calculating burning rate as a function of

⁵ Beckstead, M.W., Derr, R.L. and Price, C.F. "A Model of Composite Solid-Propellant Combustion Based on Multiple Flames," *AIAA Journal*, Vol. 8, No. 12, Dec. 1970, pp. 2200-2207.

⁶ Beckstead, M. W., "Combustion Calculations for Composite Solid Propellants," 13th JANNAF Combustion Meeting, 1976, CPIA #281, Vol. 2, pp 299-312.

⁷ Davidson, J. E. and Beckstead, M. W., "Improvements to Steady-State Combustion Modeling of Cyclotrimethylenetrinitramine", *J. of Propulsion and Power*, Vol. 13, No. 3, 1997, pp. 375-383.

⁸ Liau, Y. -C. and Yang, V., "Analysis of RDX Monopropellant Combustion with Two-Phase Subsurface Reactions", *Journal of Propulsion and Power*, Vol. 11, No. 4, 1995, pp. 729-739.

⁹ Ermolin, N. E., Korobeinichev, O. P., Tereshchenko, A. G. and Fomin, V. M., "Kinetic Calculations and Mechanism Definition for Reactions in an Ammonium Perchlorate Flame," *Combustion, Explosion & Shock Waves*, Vol 18. No. 2. pp. 61-70, Mar-Apr, 1982.

pressure and initial temperature. Generalized mechanisms have been developed and applied to many ingredients such as HMX, GAP, NG, BTTN, ADN and AP.¹⁰ The burning rates of these monopropellants vary by almost an order of magnitude, but the model calculations agree very well with experimental rate data.

The second area of recent research involves the development of codes to describe the geometrical packing of a solid propellant. The CSAR project at the University of Illinois is very active in this area with the RocPack code,^{11,12} and work at ATK/Thiokol on the ParPack code has been ongoing for some time. These models represent significant progress toward developing a realistic geometrical packing description of a solid propellant. However, combining the packing codes with a realistic flame model is still a challenge. Preliminary results by CSAR are encouraging, but obviously further work is needed. The major deficiency needing to be addressed in the CSAR model appears to be their burning rate/geometrical predictions always predicting protruding AP particles, even up to pressures as high as 136 atm. Experimental data show protruding AP up to ~40-50 atm, and recessed AP particles at higher pressures.

The third area of recent research involves coupling packing models with fundamental calculations of 2-D diffusion flames to predict burning rates of real heterogeneous propellants. A significant effort has been expended by the CSAR project, but computational limitations and the chosen kinetics model limit their progress.¹³ Their combustion model assumes a three flame model similar to the BDP model. However, their validation calculations have been limited to just four propellant formulations. CSAR predictions were within ~20-30% for three of the data sets, but were ~100% in error on the fourth. Considering the fact that there are eleven constants in CSAR's kinetic model, and they treat them as arbitrary constants, their validation is not impressive. There is a very significant need for more realistic modeling of the actual propellant combustion, using realistic chemical kinetics and models.

Very recent work at BYU incorporating realistic kinetics into a detailed numerical diffusion model shows encouraging promise towards simulating the minute detail involved in determining the burning rates of AP containing propellants.¹⁴ These results show the importance of using detailed chemical mechanisms for simulating the AP monopropellant flame, the key factor in determining propellant burning rate is reactions between the AP and binder. These reactions are dependent on both kinetics and diffusion. Both steps have to be modeled with appropriate chemistry and physics. To couple such a calculation directly into an overall motor simulation would obviously be cost prohibited. The BYU approach is to use the ATK ParPack code to realistically simulate the propellant geometry, and couple that with the BYU diffusion flame calculation and detailed kinetic mechanisms to determine the propellant burning rate. Preliminary, unpublished results look promising. This would have to be done as a sub-grid scale model calculation, generating a generalized burning rate table for each propellant that could be

¹⁰ Beckstead, M.W., Puduppakkam. K.V. and Yang, V., "Modeling and Simulation of Combustion of Solid Propellant Ingredients Using Detailed Chemical Kinetics", AIAA-2004-4036, 2004, Ft Lauderdale, Florida.

¹¹ Massa, L., Jackson, T.L., Buckmaster, J. and Campbell, M., "Three-dimensional Heterogeneous Propellant Combustion", Proc. of the Combustion Institute, 2002, 29, pp. 2975-2983.

¹² Jackson, T.L. and Buckmaster, J., "Heterogeneous Propellant Combustion," AIAA J, Vol. 40, No. 6, pp. 1122-1130.

¹³ Massa, L., Jackson, T.L. and Buckmaster, J., "New Kinetics for a Model of Heterogeneous Propellant Combustion," J. Prop. and Power, Vol. 21, No. 5, 2005, pp. 914-924.

¹⁴ Felt, S.A. and Beckstead, M.W., "A Model of the AP/HTPB Diffusion Flame", 39th JANNAF Combustion Meeting, 2003.

coupled with the overall motor simulation. This will maintain the integrity of the chemistry and physics of the combustion, allowing a reasonable computational time for the motor CFD code.

Attempting to predict a relationship between oxidizer separation distances and aluminum agglomeration potential is the fourth area of interest. Again, Jackson and Buckmaster have developed a preliminary model to simulate agglomeration.¹⁵ They calculate a “separation distance” between an aluminum particle and a large AP particle. They calibrate the separation distance by comparing their results to known data. Thus, the model is not predictive. Jackson and Buckmaster do calculate a distribution of agglomerate sizes based on the observed experimental mean agglomerate size. Again, there is a very significant need for more realistic modeling of the location of the aluminum particles relative to the large AP crystals in order to develop a predictive agglomeration model.

The current state of modeling thus appears to be headed towards a-priori predictions, based on packing codes and realistic chemical kinetics schemes. Numerical modeling is thus not yet a predictive tool, but with some effort it has the potential of developing into a useful guide to improve propellant combustion and performance.

This work will provide a significant advance in the state of the art. As discussed above very similar work is being performed at UIUC as part of the CSAR program, and is currently being published in the open literature. Their work is a very high quality from a mathematical and academic perspective, but is lacking in practical applicability. As a result, it is difficult to apply their results to practical propellants, and agreement between their calculations and practical propellant data is less than desirable. The current proposal is directed at resolving these discrepancies.

A.2.2 Formation of Aluminum/Al₂O₃ Surface Agglomerates

In addition to the burn back of the propellant surface, the size distribution and subsequent combustion of the aluminum/Al₂O₃ agglomerates leaving the surface of the propellant is a fundamental boundary condition required for simulating the solid rocket motor environment and performance. The modeling of aluminum combustion in a SRM along with predicting the trajectory of the burning aluminum/alumina droplet within the motor depends on many factors. Chief among these factors is the knowledge of the size and composition of the burning aluminum agglomerates coming off of the surface of the propellant. Also required are the rate at which these agglomerates burn, and any collision/coalescence and breakup of the droplets within the motor, see Sections 2.2.C and 2.3.

¹⁵ Jackson, T.L., Najjar, F. and Buckmaster, J., “New Aluminum Agglomeration Models and Their Use in Solid Propellant Rocket Simulations,” J. Propulsion & Power, Vol. 21, No. 5, 2005, pp. 925-936.

Determination of Aluminum Agglomerate Sizes

There are several methods for the measurement of the size and distribution of aluminum agglomerates coming off the surface of a burning propellant. These methods include film studies¹⁶, quench particles combustion bomb (QPCB) devices similar to the Pokhil device¹⁷, and combustion tank devices. Estimates of the accuracy of these methods vary from +/- 10% to 40%. Obviously, measurements require that a propellant sample exist. In many cases in the development or modification of a motor, the proposed propellants do not exist and hence models or correlations must be used to predict the agglomerate size and distribution.

There are existing models and correlations for the agglomeration process. In all versions of the SPP code¹⁸ after version 5.0, a correlation due to Dr. Robert Hermsen is used to predict agglomerate sizes when data are not available. In versions 6.0 and later of SPP, the effect of binder type was included in the agglomerate size correlation. The scatter of these correlations is larger than is acceptable even though they do represent a significant improvement over SPP 5.0, which predicted unreasonably large agglomerate sizes for high-energy propellants. However, it was concluded that experimentally determined agglomerate sizes should be input to SPP when accurate agglomerate sizes are required.

Most modern analytic models of agglomeration are usually referred to as "pocket models". The basic idea of these models is that the agglomerate forms in pockets between the AP crystals. Some of the modern agglomeration models are due to Cohen¹⁹, Kovalev²⁰, Liu²¹, Srinivas and Chakravarthy²², and Buckmaster et al.²³

While all are pocket models, the modes of mechanisms for the formation of the agglomerates are quite different. In Cohen's model the subsurface melting of the aluminum particles in the propellant along with having the volume to encapsulate the particle is the dominant factor in determining the agglomerate size. In Kovalev's model, it is assumed all of the aluminum particles that come to the surface are capable of being agglomerated. The resultant size of the agglomerate depends on the rate at which the aluminum particles come to the surface, the area defined by the pocket, and the time it takes the growing agglomerate to reach the ignition temperature. Liu's model is really a correlation based on the ideas of Gany and

¹⁶ Liu, T-K., "Experimental and Model Study of Agglomeration of Burning Aluminized Propellants," *Journal of Propulsion and Power*, vol. 21, no. 5, Sep.-Oct.. 2005, pp. 797-806.

¹⁷ Pokhil, P. F., Belyayev, et al., "Combustion of Active Metals in Active Media", FTD-MT-24-5551-73, Foreign Technology Division.

¹⁸ Nickerson, G. R., Coats, D. E., Dang, A. L., Dunn, S. S., Hermsen, R. W., "The Solid Propellant Rocket Motor Performance Computer Program (SPP), Version 6.0", Vol. I, AFRPL TR-87-078, December 1987.

¹⁹ Cohen, N.S., "A Pocket Model for Aluminum Agglomeration in Composite Propellants," AIAA-81-1585, 17th AIAA/SAE/ASME Joint Propulsion Conference, Colorado Springs, CO, July 27-29, 1981.

²⁰ Kovalev, O. B., "Motor and Plume Particle Size Prediction in Solid-Propellant Rocket Motors," *Journal of Propulsion and Power*, vol. 18, no. 6, Nov.-Dec. 2002, pp. 1199-1210.

²¹ Liu, T-K., "Experimental and Model Study of Agglomeration of Burning Aluminized Propellants," *Journal of Propulsion and Power*, vol. 21, no. 5, Sep.-Oct. 2005, pp. 797-806.

²² Srinivas, V., Chakravarthy, S.R., "Computer Model of Aluminum Agglomeration on the Burning Surface of a Composite Solid Propellant," AIAA 2005-743, 43rd AIAA Aerospace Sciences Meeting & Exhibit, Reno, NV, 2005.

²³ Buckmaster, J., Jackson, T., Massa, L., Najjar, F., and Wang, X., "The Current State of Heterogeneous Propellant Combustion Modeling," AIAA 2005-360, 43rd AIAA Aerospace Sciences Meeting & Exhibit, Reno, NV, 2005.

Caveny²⁴ and while he talks about the pocket size, the only inference to AP particle size is through the propellant burn rate. The model due to Srinivas and Chakravarthy includes a random seed packing model to keep track of the rate at which the aluminum is coming to the surface and establishes the residence time on the propellant surface by using a kinetically limited AP leading-edge flame as the aluminum ignition mechanism. The CSAR model of Buckmaster et al is simply based on the proximity of aluminum particles in the propellant as established by their random packing model. This model is without either predictive capability or the physics of the combustion process. However, it does demonstrate that packing models can supply important information concerning the agglomeration process. A major drawback in both the Cohen and Kovalev models is their reliance on average values of each mode size in multimodal AP distributions to establish the pocket size.

In our effort, we plan to use a packing model to establish the pocket size distribution for a given set of propellant constituents over a suitable length-time scale. Included in this distribution will be the amount and sizes of aluminum particles contained within each pocket. A combustion model(s) will then be proposed based on the propellant binder and oxidizers types which will establish both the residence time for agglomeration and the amount of aluminum which will meet our agglomeration criteria. One of the major inputs to this effort will be propellant surface burning data from China Lake using their new high speed digital micro-photography capability. The ability to view the agglomeration process at high pressure while also being able to distinguish the AP crystals on the propellant surface will allow for the development of improved physics models of agglomeration.

The figure below shows an example of a frame-by-frame analysis conducted for each test using Visual Fusion software. It is an example of a propellant burning in a window bomb at 30 psi, which would be similar to the proposed effort. Shown in Figure A-3, with the processed overlay, Visual Fusion tracks each particle separately and generates data on size, population and velocity. An average agglomerate size can be estimated from the flame diameter of the burning particle as they leave the propellant surface. Similarly, the particle velocity may be determined at a specified distance above the surface of the propellant.

²⁴ Gany, A., and Caveny, L. H., "Agglomeration and Ignition Mechanism of Aluminum Particles in Solid Propellants," *Seventeenth Symposium (International) on Combustion*, Combustion Inst., Pittsburg, PA 1978, pp.1453-1461.

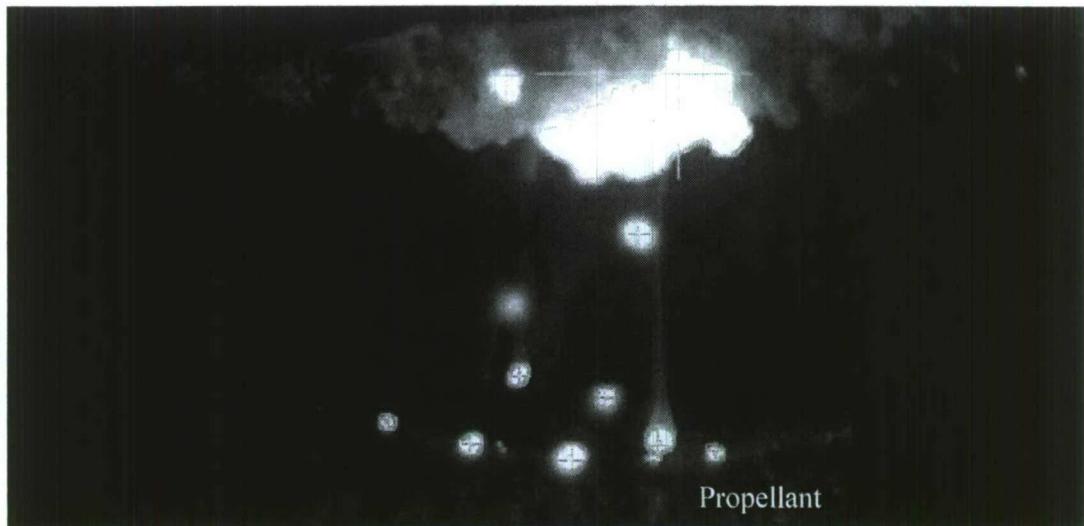


Figure A-3. Visual Fusion Results Showing the Tracked Particles and Accumulation for Propellant Burning in a Window Bomb

The questions to be answered to achieve this objective are:

1. How does the propellant constituent distribution affect the pocket size and measured agglomerate sizes?
2. How does the binder influence the residence time for agglomeration?

A.2.3 Aluminum Agglomeration Ignition and Combustion Models

It has been widely observed that the larger aluminum particles and agglomerates leave the surface of the propellant just after ignition. Hence, it is necessary to establish the ignition criteria for aluminum droplets. Most aluminum combustion models in the United States assume that ignition occurs when the oxide layer surrounding the aluminum drop melts thus, allowing the outside oxidizing gases to react with the molten aluminum droplet core. These models then assume that the droplet temperature quickly rises to the boiling point of aluminum with the flame temperature being limited by the boiling point of alumina. The latter assumption is based on the fact that alumina vapor has not been observed and hence the disassociation of alumina limits the flame temperature.

There is some disagreement about the ignition temperature of the aluminum drops. It has been postulated that the lower ignition temperatures reported by the Russians is due to binder contamination of the agglomerates which allows the surface to be breached at temperatures below the melting point of the oxide. On the other hand, Trunov and his co-workers explain the lower ignitions temperatures by “the stepwise oxidation of aluminum (that) is caused by the sequence of polymorphic phase transitions occurring in the growing oxide film”²⁵.

²⁵ Trunov, A., Schoenitz, M., and Dreizin, E. L., “Ignition of Aluminum Powders Under Different Experimental Conditions”, *Propellants, Explosives, Pyrotechnics* 30 (2005), No. 1, pp. 36-43.

Once the metal particles are ignited, the particle burning rates are known to depend on propellant composition and pressure.^{26,27,28} Significant factors are the type of oxidizer in which the metal burns (e.g., O₂, H₂O, CO₂, HF) and the oxidizer concentration, as determined by the O/F ratio of the propellant²⁹. Chamber pressure and temperature influence both, the diffusion rates of oxidizer and the heat flux to the vaporizing metal particle, as well as the type of products formed³⁰.

Aluminum Burning Models

There are at least three basic types of particle combustion models. These models include simple D² type models [HermSEN³¹, Beckstead³²], detailed engineering models [Turns et al³³, Brooks et al³⁴, and King³⁵], and full up or research models [Babuk³⁶, Liang and Beckstead³⁷]. For this effort, we have restricted our research to the first two types of models. The simple models are convenient for a wide variety of engineering applications. These applications include parametric studies of the parameters affecting incomplete combustion and 3-D CFD calculations where more complex models would be computationally prohibitive. The full up models are not practical for engineering applications even on teraflop machines. The detailed engineering model is applicable when higher fidelity solutions are warranted. A brief description of each type follows.

Simple Particle Combustion Models

Both simple particle combustion models considered are of the D² type, actually D1.8. The HermSEN and Beckstead models are similar, differing in only the oxidizing species considered and some constants. Both models take the form:

$$\frac{d(m_{Al})}{dt} = -\frac{\pi}{2} \rho_{Al} \frac{k}{1.8} D_p^3 D_p^{-1.8} \quad (2)$$

²⁶ Pokhil, P. F., Belyayev, et al, "Combustion of Active Metals in Active Media", FTD-MT-24-5551-73, Foreign Technology Division.

²⁷ Davis, A., "Solids Propellants: The Combustion of Particles of Metal Ingredients", Combustion and Flame, Volume 7, 1963, p. 359.

²⁸ Hartman, K. O., "Combustion Kinetics of Aluminum Particles in Propellant Flames," 1971 Spring Meeting of Western States Section of the Combustion Institute, Denver, Colorado.

²⁹ Micheli, P. L., "Prediction of the Burning of Aluminum in Solid Rocket Motors", presented at the Thirteenth JANNAF Combustion Meeting, Monterey, California, 13-17 September 1976.

³⁰ Brzustowski, T. A., Glassman, I., "Vapor-Phase Diffusion Flames in the Combustion of Magnesium and Aluminum", Paper 63-489, presented at the AIAA Heterogeneous Combustion Conference, Palm Beach, Florida, December 1963.

³¹ HermSEN, R. W., "Aluminum Combustion Efficiency in Solid Rocket Motors," AIAA-81-0038, AIAA 19th Aerospace Sciences Meeting, St. Louis, MO, January 12-15, 1981.

³² Beckstead, M. W., Newbold, B.R., and Waroquet, C., "A Summary of Aluminum Combustion," 37th JANNAF Combustion Meeting, CPIA No. 701, Vol. 1, November 2000, pp. 485-504.

³³ Turns, S.R., Wong, S.C., Ryba, E., "Combustion of Aluminum-Based Slurry Agglomerates", *Combustion Science and Technology*, Vol. 54, 1987.

³⁴ Brooks, K. P. and Beckstead, M. W. "Dynamics of Aluminum Combustion," *Journal of Propulsion and Power*, Vol. 11, No. 4, July-August, 1995, p. 769-780.

³⁵ King, M., "Aluminum droplet combustion", unpublished contract report for Software and Engineering Associates, Inc., 2006

³⁶ Babuk, V. A., and Vasilyev, V. A., "Model of Aluminum Agglomerate Evolution in Combustion Products of Solid Rocket Propellant", *Journal of Propulsion and Power*, Vol. 18, No. 4, July-August 2002, pp 814-823

³⁷ Liang, Y., and Beckstead, M. W., "Numerical Simulation of Unsteady, Single Aluminum Particle Combustion in Air," AIAA Paper 98-3825, 1998.

The open question in using such models is the fraction of alumina which is left on the droplet as an oxide cap.

Engineering Particle Combustion Model

A number of researchers have attempted to model aluminum combustion by analytical or numerical means. Brzustowski and Glassman³⁸ were among the first to set forth the idea of vapor-phase aluminum combustion. Their model was very similar to hydrocarbon droplet models, with two exceptions. One was the flame temperature was fixed at the boiling point of the oxide. The other was the surface temperature was fixed at the boiling point of aluminum.

Several years later, Law³⁹ expanded the work of Brzustowski and Glassman by developing a model that included the diffusion of combustion products from the flame zone back to the particle surface, as well as an infinitely thin condensation zone (infinitely fast condensation rate). Later, Law and Williams⁴⁰ modified the model to include an extended flame zone. Law's first steady-state model works reasonably well for oxygen-containing atmospheres. However, it lacks the ability to incorporate multiple oxidizers and their products, oxide accumulation on the particle surface, and convection.

Turns et al, Brooks, and King have all developed aluminum combustion codes based on modifications to Law's model. These models allow for the effects of an accumulating oxide cap, variable transport properties, as well as multiple oxidizers. The models also allow for both water and CO₂ as oxidizers (in addition to oxygen). Each oxidizer has been shown to have a different effect on burning time. The effect of the oxide cap is to decrease the burning rate as the oxide accumulates due to a reduced surface area, leading to an exponent of ~1.7-1.8 in the D2 approach. Brooks' results compared favorably with a limited range of experimental data, but needs to be explored for a wider range of conditions with motor-like environments. King's model needs to be evaluated against data. Calculation times for both Brooks' and King's models are very short, so they are logical candidates for incorporation into our proposed code.

A somewhat simpler ignition and aluminum combustion model has been proposed by DesJardin and his co-workers.⁴¹ The model is more simplistic than those described above and has only been checked out for aluminum burning in air. However, the model does include an ignition model and might be suitable for a back-up position if problems arise in implementing either Brooks' or King's model.

One of the above aluminum combustion models will be the starting point for studying metal combustion in a solid propellant motor environment. An area where further study is needed is in cloud combustion characteristics. Studies of dense sprays indicate that for particle

³⁸ Brzustowski, T.A. and Glassman, I. "Spectroscopic Investigation of Metal Combustion," *Heterogeneous Combustion*, Vol. 15, AIAA, New York, 1964, p. 41-73.

³⁹ Law, C. K. "A Simplified Theoretical Model for the Vapor-Phase Combustion of Metal Particles," *Combustion Science and Technology*, 1973, Vol. 7, p. 197-212.

⁴⁰ Law, C. K., and Williams, F.A. "On a Class of Models for Droplet Combustion," AIAA Paper 74-147, Jan. 1974.

⁴¹ DesJardin, P.E., Felske, J.D., Carrara, M.D., "Mechanistic Model for Aluminum Particle Ignition and Combustion in Air", *Journal of Propulsion and Power*, Vol. 21, No. 3, May-June 2005, pp 478-485.

cloud densities typical of those in solid propellants, there are almost certainly interactions between burning particles. Calculations indicate that for metal concentrations of ~10% the extended flames of individual particles most likely overlap, modifying the outer boundary conditions experienced by the particles. As part of this program, these conditions will be explored and incorporated into the selected engineering model.

Thermochemistry

The amount of available oxidizer is an important parameter in computing the burning rate of the aluminum particles. The simplest approach to computing the rate at which the oxidizer is being depleted by the burning aluminum is to assume chemical equilibrium in the motor cavity. In general, this assumption is an excellent one for the chamber flowfield.

Equilibrium thermochemistry in general requires the elemental composition and two independent thermodynamic state variables to define everything else. The computation of the elemental composition within the flow field is straight forward if the Shvab-Zel'dovich formulation is used⁴², however it is also very time consuming. A simpler approach used with some success at SEA on our IHPRT work is to simulate the effect of the combustion of aluminum on the elemental composition by carrying along as a parameter the amount of combusted or burned aluminum. This assumption allows us to define the elemental composition in terms of the amount of burned aluminum and overall propellant composition. Hence, we can compute any scalar quantity, ϕ , from:

$$\phi = \phi ([\text{Al}], h, P)$$

where $[\text{Al}]$ is the amount of burned aluminum, h = gas phase static enthalpy, and P = pressure.

The function ϕ represents an interpolation algorithm in the three independent variables. For multiple propellants, a parameter specifying the amounts of each propellant has to be added to the list of independent variables of the function, ϕ .

The questions to be answered from this objective are:

1. What are the criteria for the selection of the ignition model?
2. How important are particle cloud effects on the droplet burning rate?
3. What are the computational requirements for the various models?

A.3 Modeling Approaches

The AFRL Modeling and Simulation Program focused significant effort on developing a multi-dimensional, multiphase CFD approach for solid rocket environment and performance modeling. This work was built on previously funded efforts by the Air Force, such as the development of the multi-physics computer code CEL-MINT.⁴³ While the commercial code FLUENT was used by ATK extensively in the Modeling and Simulation program, it is recognized that CFD and multi-physics modeling is a rapidly evolving field. A review of

⁴² Kuo, K. K., *Principals of Combustion* 2nd Ed., John Wiley & Sons, Inc., New Jersey, 2005, pp. 333-336.

⁴³ Sabnis, J.S., F.J. de Jong, and H.J. Gibeling. "A two-phase distributed combustion model for metalized solid propellants", 28th JANNAF Combustion Meeting, San Antonio, TX, October, 1991.

commercial code technologies available such as FLUENT, CFD++, as well as other CFD codes, will be performed to choose the most viable platform for incorporating the particle packing and combustion models. In addition, droplet trajectory predictions in the motor environment require two additional sub-models.

A.3.1 Collision/Coalescence and Fragmentation/Breakup Model

We propose to look at a variety of collision/coalescence models. One approach is to modify the collision efficiency model as used by Salita⁴⁴ and/or Friedlander⁴⁵ with the model of Brazier-Smith et al or, Ashgriz and Poo. Both, the Brazier-Smith et al⁴⁶ and Ashgriz and Poo⁴⁷ models have better comparisons to data than the Friedlander model. However, neither model has been validated with droplet data for dissimilar surface tensions.

The Fragmentation/Breakup Model currently used by most of the IHPPT M&S modelers is based on the concept of a critical Weber number and predicts that the droplets will fragment when the Weber number is as follows, $We = D_p \rho V^2 / \sigma > 4CD_0$. This is basically the approach of Bartlett and Delaney⁴⁸ and Kovalev⁵. The table below outlines the observed breakup with Weber number. It is usually assumed that the first mode is experienced in a solid propellant rocket motor.

Table A-2. Observed Breakup with Respect to the Weber Number

Breakup Mode	Weber number, $We = D_p \rho V^2 / \sigma$
Vibrational Breakup	$We < 12$
Bag Breakup	$12 < We < 50$
Bag and Stamen Breakup	$50 < We < 100$
Sheet Stripping	$100 < We < 350$
Wave Crest Stripping	$We > 350$

Another approach that will be investigated is the Rayleigh-Taylor breakup model that determines how and when droplets will breakup by predicting the wavelength of the fastest growing disturbances. The disturbances for the Rayleigh-Taylor model are due to acceleration instabilities on the droplet surface rather than aerodynamic instabilities (Patterson and Reitz, 1998)⁴⁹. These models will be reviewed to find out which model gives a better fit to known data.

The questions to be answered from this objective are:

⁴⁴ Salita, M., "Simulation of A1203 Collision/Coalescence Using Water and Mercury Droplets", Thiokol TWR-40224, 5/18/89; also 26th JANNAF Combustion Meeting (JPL), 10/89.

⁴⁵ Friedlander, S. K., *Smoke, Dust, and Haze*, Wiley, 1977, pp. 88-121.

⁴⁶ Brazier-Smith, P. R., Jennings, S. G., and Latham, J., "The Interaction of Falling Water Drops: Coalescence", *Proc. Royal Soc. of London, Series A*, Vol. 326 (1972), pp. 393-408.

⁴⁷ Ashgriz, N. and Poo, J. Y., "Coalescence and Separation in Binary Collisions of Liquid Drops", *J. Fluid Mech.*, Vol. 221, pp. 183-204, 1990.

⁴⁸ Bartlett, R.W., and Delaney, L.J., "Effect of Liquid Surface Tension on Maximum Particle Size in Two-Phase Nozzle Flow", *Pyrodynamics*, 4, 337-341 (1966).

⁴⁹ Patterson, M. A. and Reitz, R. D., "Modeling the Effects of Fuel Spray Characteristics on Diesel Engine Combustion and Emissions", SAE paper 98-0131, (1998).

1. What collision/coalescence model should we use?
2. What fragmentation/breakup model should we use and how do we determine the parameters required by the model?

A.4 Review and Select Models of Droplet Impact, Erosion, and Heat Transfer

One of the more important reasons for tracking the trajectories of burning aluminum particles in the motor is to assess the damage that the particles do to the internal insulation and nozzle wall on impact. The damage can manifest itself in several ways. First there is mechanical removal of material, secondly there is thermal shock and resultant stress from the direct transfer of energy from the molten drops to the surface, and thirdly there are thermochemical reactions and ablation of the nozzle material. All of the above phenomena can lead to insulation or nozzle failure.

As part of an Air Force sponsored investigation into a nozzle failure, Hylin, Coats, and Dunn⁵⁰ of SEA reviewed the literature concerning alumina impingement and modeling. This work has been extended by the Thermal Working Group of the AFRL sponsored IHPRT Modeling and Simulation effort of which Aerojet, ATK-Thiokol, and SEA are participants. Nickerson⁵¹ as part of the Thermal Working Group has developed simplified diffusion limited erosion models for the reactions of both molten aluminum and alumina with carbon wall materials. The key chemical reactions between carbon and aluminum/alumina have been identified which is a major step in being able to predict the thermochemical erosion of the nozzle wall. In addition, SEA as part of a Navy sponsored SBIR effort on gun tube erosion has developed a generalized capability to treat diffusion limited thermochemical erosion in combustion environments.⁵² The application of the flowfield and combustion technology being developed as part of this proposed effort coupled with SEA's generalized erosion capability should give us the ability to accurately compute the impact on nozzle materials in SRM's.

While particle drag and heat transfer models are fairly well developed, treating the effect of burning droplets on the drag coefficient needs to be evaluated. As does the impact of turbulence models on the amount and velocity of the drops impacting the nozzle wall.

The effort on this task in Phase I will deal with the review and selection of models which will be incorporated into the Phase II computer program. ATK has already developed computational approaches as part of the Air Force Modeling and Simulation program to characterize in-depth thermo-chemical erosion of ablating materials in a computer code called HERO. At present, HERO is a two-dimensional code that models the in-depth heating and decomposition of ablating materials, the transport of generated pyrolysis gas products through the developing char layer, and the thermochemical and/or mechanical removal of the char at the surface. Through the FEM-builder interface, HERO can also be coupled with CFD-based

⁵⁰ Hylin, E. C., Coats, D. E., and Dunn, S. S., "Alumina Impingement Literature Review and Analysis", AFRL-PR-ED-TR-2003-0038, Oct. 2003.

⁵¹ Nickerson, G. R., "The Chemical Erosion of a Carbon Surface by Molten Aluminum or Aluminum Oxide", Nickerson and Associates, Inc. Memo, May 2005.

⁵² Dunn, S. S., "Modeling High-Temperature Erosive Gas Flow to Support Barrel Erosion Reduction Concept Modeling for Fire Support Gun Application" Final Report, N00178-03-C-1010, August 2005.

environment prediction models in a comprehensive solution strategy. As a companion sub-model, ATK has also developed a slagging model to capture the specific heating mechanism of slag impinging on a surface. This model simulates the effects of both slag cooling to the point of freezing on a cold surface, and subsequent heating and remelting of the slag layer.

The questions from this objective to be answered are:

1. Are the flowfield and droplet drag models as suggested by the IHPPT M&S effort adequate for this effort?
2. Are there better thermochemical ablation models than those already identified?
3. What level of erosion modeling is required for this effort?

A.5 Review and Select the Computer Framework Software Programs in which the Physical Models will be Implemented

One of the more critical tasks in this effort is to select the computer software framework in which the models developed will work. It is clear that writing a code from scratch is well beyond the scope of this program. Hence an existing 3-D flow solver will be used. There are basically two approaches that we can follow; the first is to use a commercially available code such as Fluent or CFD++ as mentioned in 2.3. The second approach would be to use a rocket motor application specific code such as SPP. Both methods offer substantial benefits. The use of commercial codes assures continued support and increasing capability especially as it pertains to numerical methods and taking advantage of new hardware capabilities. On the other hand, application specific codes (ASC) have a framework which encompasses the entire application, in our case, SRMs. Commercial codes have high yearly per seat costs while ASC's do not. For example, a perpetual SPP site license is less than a single seat for Fluent for a single year. If the product developed under this effort is not affordable and reasonably easy to use, it will not be used by industry. For example, the CELMINT code which AFRL paid for the development of in the mid 90's only has one non-developer user, Harold Whitesides of ERC, in the entire country.

Both ATK and SEA have significant expertise and experience in developing software frameworks for predicting solid rocket motor environments and performance. ATK has developed the FEM-BUILDER code under contract with the Air Force, which has been specifically designed to couple computer codes from different disciplines (fluid dynamics, heat transfer, structures) into an overall computational framework for the simultaneous solution of multi-physics problems.

Analyses of solid rocket motors must be performed at different times during the burn. This requirement means that the boundaries of the CFD computational domain will change significantly with time. A method of automatically gridding the motor cavity at different web steps is necessary if the code is to be easy to use. Both SEA with its SPP code and ATK with their FEM-BUILDER code have this capability. The SEA code and its automatic gridding capability are described below.

SEA's gridding process can be performed on a solid rocket motor at any time during the burnback. The generated grid represents the remaining interior volume of the motor, allowing a quasi-steady-state CFD analysis of a motor to be performed at various burn times.

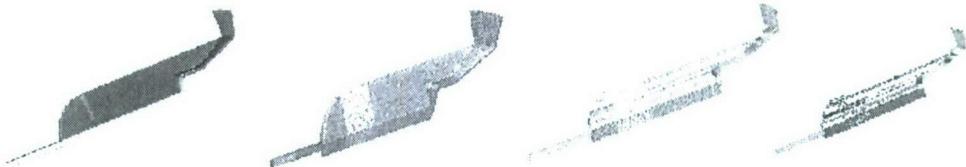


Figure A-4: Steps in Automated Grid Generation Process

SEA's CFD analysis program is currently a 3D Euler flow solver; it is being extended as part of a Navy effort to become a Navier-Stokes solver. In Figure A-5, a vortex has been captured after a sudden expansion in the aft end of a tactical motor.



Figure A-5: Rotational Flowfield Example

A major development focus at this time is to reduce both user time and CPU time required for convergence. User time is addressed by automating the process of grid generation and CFD input setup from an SPP input file to a CFD grid and input file as previously discussed. CPU time is addressed with two methods. The first is code parallelization and optimization, and the second is grid sequencing. An example of grid sequencing is shown in Figure A-6.



Figure A-6: Grid Sequencing Example

Currently, the SEA/ATK/BYU team is planning to evaluate both the use of SEA's SPP and ATK's FEM-Builder code as the overall framework code in which this software will be distributed. ATK has agreed to the licensing of both their ParPack and FEM-Builder software if this effort goes to completion.

The questions to be answered for this objective are:

1. Which type of code should be used for the flowfield solver?
2. How will all of the models be tied together?
3. How can we fit a Graphical User Interface over the resultant code?

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APPENDIX B: PHASE I WORK PLAN

The Phase 1 work plan is designed to demonstrate the feasibility of the proposed innovation. Each Task has been fashioned to answer the respective questions asked in the Technical Objectives section. Task 1 will address packing model requirements. Task 2 will try to identify possible agglomeration models or approaches that can be used to predict the size, density, and velocity of the agglomerates coming off the surface of the propellant. The third task will investigate different models which might be used to burn the resulting agglomerates. Task 4 reviews the collision/coalescence and breakup models which will be used. Task 5 will either select or lay out the criteria for selection of the CFD solver and the computer framework software to be used in the final product. The final task, Task 6, will document the effort performed under this contract.

B.1 Propellant Constituent Packing Model (ATK Task)

The ATK packing model, PARPACK, already contains the features needed to meet the goals of this proposed effort in regards to mechanical properties. This capability will be demonstrated as part of the feasibility study. However, with respect to agglomerate modeling, the code will need to be exercised to provide the input and insight needed to develop a surface agglomeration model. To this end, the following sub-tasks are required.

Task 1, Propellant Constituent Packing Model (ATK Task)

The ATK packing model, PARPACK, already contains the features needed to meet the goals of this proposed effort in regards to mechanical properties. This capability will be demonstrated as part of the feasibility study. However, with respect to agglomerate modeling, the code will need to be exercised to provide the input and insight needed to develop a surface agglomeration model. To this end, the following sub-tasks are required.

Task 1.1, Aluminum Distribution and Pocket Statistics

- Compare predicted pack morphology with measured agglomerate size distributions for several propellants with a wide variety of agglomeration propensities.
- Confirm and quantify pack micro-geometric effects on aluminum pockets and their expected enhancement of large agglomerates.
- Unite packing code with agglomeration and combustion codes so they seamlessly feed the necessary micro-geometric information to them

Task 1.2 Transfer packing code to SEA code suit

The PARPACK object code will be handed off to SEA for use in the surface agglomeration model selection, Task 2.2.

Task 2, Combustion Models (SEA/BYU/ATK Task)

This task addresses the need for a propellant burnback model, a surface agglomeration model, and an aluminum droplet burning model.

Task 2.1 Burn Back of the Propellant Surface (BYU Task)

Task 2.1.1

Initially, this task will focus on coupling the BYU detailed kinetics code with PARPACK to evaluate the geometrical effects of particle size distributions without the effects of diffusion flames. Parallel work will be initiated to optimize the diffusion flame code for later coupling with PARPACK. Initial validation data will be Miller's non-aluminized propellant data set (~20 formulations).

Eventually, this effort will focus on evaluating the geometrical effects of particle size distributions on burning rate using an initial diffusion flame analysis coupled with the main code. The diffusion flame code will be run as a sub-grid model, varying pertinent parameters to develop correlations that can be coupled into the main code. The validation data will come from both Miller's non-aluminized and aluminized propellant data sets.

Task 2.1.2

The agglomeration task will focus on using PARPACK to calculate separation distances for the large AP crystals in a formulation. Different definitions of separation distance will be explored to determine a viable algorithm. These calculations will be compared to available data (i.e. initially the shuttle formulation, and others that are available in the literature).

Eventually, the agglomeration task will develop a definitive separation distance algorithm for coupling into the main code. Validation data will come from parallel programs utilizing rotating quench bomb results for ATK propellants and high resolution micro-cinematography data from China Lake.

Task 2.2, Aluminum Agglomeration Model Selection (SEA/BYU/ATK Task)

Part of the model selection task has already been addressed in Task 2.1.2. Both the PARPACK and ROC PACK packing models will be used to define pocket volumes or characteristic distances in terms of AP sizes and distributions. The first step is to look at monomodal distributions with small standard deviations and compare the results to average pocket volumes. Following this study, we will look at bimodal and trimodal distributions with varying standard deviations to understand the statistics of aluminum size and content in the pockets which come to the surface of the burning propellant. The results of this study will be compared to quench bomb data taken by Aerojet and ATK as part of the IHPPT M&S effort. This part of the task will address the question: How does the propellant constituent distribution affect the pocket size and measured agglomerate sizes?

As part of this task we will work with Alice Atwood at China Lake to take pictures and measurements of at least a monomodal propellant sample. We will also lay out an experimental program for the Phase II effort where both distributions and binder formulations are varied. It is this effort that will answer the question: How does the binder influence the residence time for agglomeration?

While final selection of an agglomeration model will come in Phase II, we should have enough information in the Phase I effort to lay out the final model selection criteria.

Task 2.3, Aluminum Agglomerate Burning Rate Model Selection (BYU/SEA Task)

The first step in determining an aluminum combustion model is selecting an ignition mechanism and temperature. To this end, the current literature will be reviewed and the most promising models and data investigated. In particular, the models of Turnov et al and DesJardin et al will be reviewed along with a search of the latest Russian literature. In the event that there is no clear choice, the top two most likely models will be coded up and tested for suitability in the proposed Phase II models. The criteria for the model selection will be based on the availability of the required input, suitability for inclusion in a larger CFD model, and comparison to available data. This effort will answer the question: What are the criteria for the selection of the ignition model?

As a matter of computational practicality, simple particle combustion models considered of the D^2 type will be incorporated into the proposed code. Either the Hermsen or the Beckstead model will be chosen based on the experiences gained from the Air Force IHPPT M&S contract work. The real question is whether a more complete model with higher physical fidelity can be included in a CFD model without making the computer run time impractical. The existing Brooks model, available through BYU, and existing King model, available through SEA, will be tested for speed and accuracy against available data and against the empirical models. Depending on the results of these tests, either one or both of these models will be selected for the Phase II effort. The question to be answered from this objective is: What are the computational requirements for the various models?

All of the above models are single droplet models. The boundary conditions for these models assume not only spherical symmetry but that there are uniform conditions far from the drop. The number density of the burning droplets is high enough that numerous drops will be close enough for interaction between droplets, even though the average separation distance of drops of the same size is not small. We will test the sensitivity of the droplet burning rate to changes in the boundary conditions by running various tests in which we modify the far field boundary conditions. The question to be answered from this objective is: How important are particle cloud effects on the droplet burning rate?

Task 3, Review and select droplet coalescence/breakup models along with droplet ballistic trajectory models. Also review CFD solvers as vehicles into which to incorporate the models. (SEA/ATK Task)

The first step in this task is to review the work done and models selected in the AFRL sponsored IHPPT M&S program. If this work shows essentially no difference between the various models selected by Aerojet, ATK, and SEA, then the simplest model with reasonable physics will be selected. However, if there are significant differences, then we will use SEA's IHPPT M&S developed combustion efficiency code as a test bed to check out the various models. We shall also review the literature for data to test out the model, paying special attention to data which treats drops of unlike materials.

The SEA/BYU/ATK team will also conduct a comparison of the various CFD flowfield solvers used in the solid rocket motor community.

Task 4, Review and select models of droplet impact, erosion, and heat transfer. (ATK/SEA Task)

There has been a significant effort by both ATK and SEA on insulation and nozzle erosion in the AFRL sponsored IHPPT M&S effort as discussed in the Technical Objective section. This work as well as a current literature search will be review for inclusion into the Phase II computer program.

This review will answer the following questions:

- i. Are the flowfield and droplet drag models, as suggested by the IHPPT M&S effort, adequate for this effort?
- ii. Are there better thermochemical ablation models than those already identified?
- iii. What level of erosion modeling is required for this effort?

Task 5, Review and select the computer framework software programs in which the physical models will be implemented. (SEA/ATK Task)

Both the SPP and FEM-BUILDER codes offer a suitable framework for the aluminum combustion and flow solver models. This task is designed to review the possibilities, both commercial and technical, of using either or both of these codes in the finished Phase II product. SEA will explore with ATK the licensing potential of both the FEM-BUILDER and PARPACK codes with hooks to CFD solvers such as FLUENT or CFD++. ATK has already agreed to the licensing of its PARPACK technology as part of this effort.

The initial design of the Graphical User Interface (GUI) will be laid out as part of this task. The design will reflect the choice or choices of the framework software selected.

Task 6, Program Documentation (SEA/BYU/ATK Task)

The purpose of this task is to document the work performed under the first 5 tasks. The documentation will consist of a final report on the work which was performed, the data generated, and the results obtained. The final report will be the product delivered from the Phase I effort.

If the feasibility of the innovation is shown, the documentation will also act as a blueprint for the Phase 2 effort. The tasks listed in Section 3 will be performed in accordance with the schedule shown in Figure B-1.

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Tasks	Months after Contract Initiation									Staff Assigned
	1	2	3	4	5	6	7	8	9	
1 Propellant Constituent Packing Model	X	X	X							Davis
2 Combustion Models										
2.1 Propellant Burnback Model		X	X	X	X	X	X			Beckstead
2.2 Surface Agglomeration Model			X	X	X	X	X	X		Hylin/Beckstead
2.3 Al Burning Rate Model Selection					X	X	X			Hylin/Beckstead
3 Review and Select Droplet Models				X	X	X				3.1.1.1.1 Hylin/ Eaton
4 Review and Select Models of Droplet Impact, Erosion, and Heat Transfer					X	X	X			Hylin/Eaton
5 Review and Select the Computer Framework					X	X	X	X		Hylin/Eaton
6 Final Report Preparation								X	X	Hylin/Beckstead/ Davis

Figure B-1. Performance Schedule

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APPENDIX C: PROGRESS REPORT #1

SN285

Contract Progress, Status, and Management Report

FA9550-06-C-0069

**Aluminum Agglomeration and Trajectory
in Solid Rocket Motors**

**Contractor's Status Report No. 1
For August - October 2006**

November 2006

WARNING – This document contains technical data whose export is restricted by the Arms Export Control Act (Title 22, U.S.C., Sec 2751 et seq.) or the Export Administrations act of 1979, as amended. (Title 50, U.S.C., App. 2401, et seq.) Violations of these export laws are subject to severe criminal penalties.

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Progress for the Period August - October 2006

C.1 General

Most of the work during this reporting period was done on the various aluminum droplet models, Tasks 2 and 3.

C.2 Schedule

The Program Schedule is shown below.

Table C-1. Program Schedule

Tasks	Months after Contract Initiation									Staff Assigned
	1	2	3	4	5	6	7	8	9	
1 Propellant Constituent Packing Model	X	X	X							Davis
2 Combustion Models										
2.1 Propellant Burnback Model		X	X	X	X	X	X			Beckstead
2.2 Surface Agglomeration Model			X	X	X	X	X	X		Hylin/Beckstead
2.3 Al Burning Rate Model Selection					X	X	X			Hylin/Beckstead
3 Review and Select Droplet Models				X	X	X				Hylin/Eaton
4 Review and Select Models of Droplet Impact, Erosion, and Heat Transfer					X	X	X			Hylin/Eaton
5 Review and Select the Computer Framework					X	X	X	X		Hylin/Eaton
6 Final Report Preparation								X	X	Hylin/Beckstead/ Davis

C.3 Progress by Task*C.3.1 Task 1. Propellant Constituent Packing Model*

An intellectual property rights agreement was signed with ATK Thiokol making the ATK propellant constituent packing model available to SEA and BYU. Also, SEA obtained the ROCPACK model from UIUC.

C.3.2 Task 2. Combustion Models

C.3.2.1. Task 2.1. Propellant Burnback Model

The literature is being reviewed on various burn back models.

C.3.2.2. Task 2.2. Surface Agglomeration Model

Surface agglomeration models are being reviewed for inclusion into this model. The models reviewed are due to Cohen¹, Hermsen², and Liu³ as well as the latest model due to Jackson et al⁴. In addition, we have received but not reviewed the Russian paper by Yagodikov et al⁵

C.3.2.3 Task 2.3. Al Burning Rate Model Selection

The analytical burn rate models of King⁶, Turns⁷, and Law⁸ are being reviewed. The empirical models of Hermsen⁹ and Beckstead¹⁰ are also being reviewed.

C.3.3 Task 3. Review and Select Droplet Models

Our general approach to modeling the droplet phases will be to select a set of droplets, of varying sizes and compositions, each of which will be *representative* of a group of similar droplets. Calculations may then be carried out for these representative droplets and subsequently aggregated to form a description of the droplet phase(s) as a whole. This is the same general framework as that which has been successfully used in codes such as SPP [DCF-2005a, DCF-2005b] and OD3P. Particular physical phenomena may then be described by sub-models, each of which is defined with respect to its actions on and between the various representative droplets. Physical phenomena of principal interest include droplet agglomeration and breakup (fragmentation). Other physical phenomena include evaporation/condensation, solidification, and material density change.

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- ¹ Cohen, N.S., "A Pocket Model for Aluminum Agglomeration in Composite Propellants," AIAA-81-1585, 17th AIAA/SAE/ASME Joint Propulsion Conference, Colorado Springs, CO, July 27-29, 1981.
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- ⁶ King, M., "Aluminum droplet combustion", unpublished contract report for Software and Engineering Associates, Inc., 2006
- ⁷ Turns, S.R., Wong, S.C., Ryba, E., "Combustion of Aluminum-Based Slurry Agglomerates", *Combustion Science And Technology*, Vol. 54, 1987
- ⁸ Law, C. K., and Williams, F.A. "On a Class of Models for Droplet Combustion," AIAA Paper 74-147, Jan. 1974.
- ⁹ Hermsen, R. W., "Aluminum Combustion Efficiency in Solid Rocket Motors," AIAA-81-0038, AIAA 19th Aerospace Sciences Meeting, St. Louis, MO, January 12-15, 1981.
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C.3.3.1 Droplet Agglomeration Model

The model adopted for droplet agglomeration is the collision + coalescence model that was used in the OD3P code, as modified and improved by Salita [S-1989]. Fundamental to this model is the agglomerating volume flowrate, expressed as

$$\dot{V}_{jk} = \eta_a(j, k) \pi [R_j^2 + R_k^2] \sqrt{(\mathbf{V}_j - \mathbf{V}_k) \cdot (\mathbf{V}_j - \mathbf{V}_k)}.$$

The right-hand side of this expression comprises the product of an agglomeration efficiency η_a , the collision cross-section, and the relative velocity between the two representative groups of particles. The agglomeration efficiency is itself expressed as the product of a collision efficiency and a coalescence efficiency:

$$\eta_a(j, k) = \eta_{coll}(j, k) \eta_{coal}(j, k).$$

For the collision efficiency we use the expression given by Salita [S-1989]:

$$\eta_{coll}(j, k) = \left[1 + \frac{1.262 + 0.0457 (z \text{Re})^{0.782}}{\text{St}^{1.26} + 4\pi z^2} \right]^{-1}.$$

The various terms in this expression are defined as follows:

$$\begin{aligned} z &= \frac{R_s}{R_L}, \quad R_s = \min(R_j, R_k), \quad R_L = \max(R_j, R_k); \\ \text{Re} &= \frac{\rho_{gas} |\mathbf{V}_{gas} - \mathbf{V}_L| 2R_L}{\mu_{gas}}; \\ \text{St} &= \left(\frac{2}{9} \right) \frac{\rho_{mp} |\mathbf{V}_{gas} - \mathbf{V}_L| R_s^2}{\mu_{gas} R_L} = \left(\frac{1}{9} \right) \text{Re} \left(\frac{\rho_{mp}}{\rho_{gas}} \right) z^2. \end{aligned}$$

Here the subscript S refers to the smaller of the two particles, while the subscript L refers to the larger. The gas/particle velocity difference appearing in the preceding equations is defined as

$$|\mathbf{V}_{gas} - \mathbf{V}_L| = \sqrt{(\mathbf{V}_{gas} - \mathbf{V}_L) \cdot (\mathbf{V}_{gas} - \mathbf{V}_L)}.$$

For the coalescence efficiency, we follow Brazier-Smith, Jennings, and Latham [BJL-1972]:

$$\eta_{coal}(j, k) = \left(\frac{12}{5}\right) \frac{1}{We_s} F(z),$$

in which

$$We_s = \frac{R_s \rho_{mp} |\mathbf{V}_s - \mathbf{V}_L|^2}{\sigma}$$

and

$$F(z) = \frac{(1+z^3)^{1/3}}{z^5 (1+z)^2} \left[1 + z^2 - (1+z^3)^{2/3} \right].$$

The velocity difference appearing above is defined as

$$|\mathbf{V}_s - \mathbf{V}_L| = \sqrt{(\mathbf{V}_s - \mathbf{V}_L) \cdot (\mathbf{V}_s - \mathbf{V}_L)} = \sqrt{(\mathbf{V}_j - \mathbf{V}_k) \cdot (\mathbf{V}_j - \mathbf{V}_k)}.$$

Salita [S-1991] has demonstrated the applicability of these formulae to Al₂O₃ droplets.

Advantages of this approach are that the models for the collision efficiency and the coalescence efficiency are independent, and furthermore that their individual definitions do not affect the implementation of the rest of the agglomeration model. Thus we are free to later substitute a more comprehensive and accurate expression for, say, the coalescence efficiency. In that particular regard, we note that in lieu of or in addition to the model of Brazier-Smith, Jennings, and Latham [BJL-1972], we may use ideas from the more recent model of Ashgriz and Poo [AP-1990].

C.3.3.2 Droplet Breakup Models

At this point, we are considering two alternative models for droplet fragmentation. One simply assumes that fragmentation occurs instantaneously when a critical Weber number for the droplets is exceeded. The other is the Taylor Analogy Breakup (TAB) model first described by O'Rourke and Amsden [OA-1987]. Additional models may be considered in the future. Ease of implementation, stability, and the reasonableness and accuracy of the predictions must all be considered in the process of model selection.

The criterion for breakup in the Weber-number model is

$$\frac{2R\rho_{gas} |\mathbf{V}_p - \mathbf{V}_g|^2}{\sigma} > \text{We}_{\text{crit}},$$

in which R is the droplet radius, ρ_{gas} is the gas-phase density, $|\mathbf{V}_p - \mathbf{V}_g|$ is the magnitude of the difference between the droplet and gas-phase velocities, σ is the surface tension of the droplet, and We_{crit} is some critical value. It is assumed that at the instant when the above criterion is met, the droplet instantaneously fragments into n smaller droplets of equal size. This model considers the balance between aerodynamic forces and surface tension forces acting on a droplet, and assumes that breakup occurs when the former sufficiently exceed the latter.

Noting that viscous forces within a droplet or between the droplet and gas may also influence droplet fragmentation, Hylin and Salita [HS-2006] speculate that a more general criterion for breakup might be expressed in terms of the Ohnesorge number,

$$Z = \frac{\mu_{mp}}{\sqrt{\rho_{mp} R \sigma}},$$

and either the Capillary number,

$$\text{Ca} = \frac{|\mathbf{V}_p - \mathbf{V}_g| \mu_{gas}}{\sigma},$$

or the droplet Reynolds number,

$$\text{Re} = \frac{2R\rho_{gas} |\mathbf{V}_p - \mathbf{V}_g|}{\mu_{gas}},$$

in addition to the Weber number. This idea has not yet been explored.

With any model that assumes instantaneous droplet fragmentation, if we try to represent the fragmentation locus at discrete sample points (such as finite-difference grid points or finite-volume or finite-element cell centers), we face the issue of *aliasing*. By assumption, the fragmentation locus is an infinitely thin curve or surface, while the grid points or cell centers are spaced a finite distance apart. Consequently, the true locus will generally pass *between* grid-points; but if the droplet radii are simply set to a pre-fragmentation (R) or a post-fragmentation ($R / n^{1/3}$) value at the grid points, then the locus as represented on the grid will generally exhibit a stair-stepped, jagged appearance. In signal- and image-processing problems, this kind of aliasing can be dealt with by means of an appropriately constructed linear filter [L-1997, FVFH-1990]. However, the filtering of a quasi-linear dynamical system such as the droplet Euler equations is more problematic.

C.3.3.3 Droplet Model References

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C.4 Task 4. Review and Select Models of Droplet Impact, Erosion, and Heat Transfer

This task has not started yet.

C.5 Task 5. Review and Select and Computer Framework

This task has not started yet.

C.6 Management and Cost

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C.6.1 Progress

The contract is on schedule and we are reviewing our program plan to make sure that all elements of it are on track.

C.6.2 Management

There were no management issues during this reporting period.

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APPENDIX D: PROGRESS REPORT #2

SN285

Contract Progress, Status, and Management Report

FA9550-06-C-0069

**Aluminum Agglomeration and Trajectory
in Solid Rocket Motors**

**Contractor's Status Report No. 2
For November 2006 - January 2007**

February 2007

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D.1 General

The work done during this reporting period included progress on most of the tasks. Work on Task 3, the review and selection of droplet models, is nearly complete. The other tasks are all well under way, with the exception of Task 1, the propellant constituent packing model. ATK/Thiokol's ParPack code is fully developed, but the means of integrating it with the other aspects of the current problem have not yet been worked out. In spite of this, work on Task 2 has been able to proceed. Some of the pending work on Task 4 and Task 5 may require further coordination between SEA and ATK/Thiokol.

D.2 Schedule

The Program Schedule is shown below. Task 1 is behind schedule, but this is offset by Task 3 being ahead of schedule. The other tasks are proceeding as originally planned.

Table D-1. Program Schedule

Tasks	Months after Contract Initiation									Staff Assigned
	1	2	3	4	5	6	7	8	9	
1 Propellant Constituent Packing Model	X	X	X							Davis
2 Combustion Models										
2.1 Propellant Burnback Model		X	X	X	X	X	X			Beckstead
2.2 Surface Agglomeration Model			X	X	X	X	X	X		Hylin/Beckstead
2.3 Al Burning Rate Model Selection					X	X	X			Hylin/Beckstead
3 Review and Select Droplet Models				X	X	X				3.1.1.1.2 Hylin/Eaton
4 Review and Select Models of Droplet Impact, Erosion, and Heat Transfer					X	X	X			Hylin/Eaton
5 Review and Select the Computer Framework					X	X	X	X		Hylin/Eaton
6 Final Report Preparation								X	X	Hylin/Beckstead/Davis

D.3 Progress by Task

D.3.1 Task 1. Propellant Constituent Packing Model

In January, Dr. Hylin and Mr. Coats of SEA met with Dr. Davis of ATK/Thiokol and Dr. Beckstead of BYU to discuss the physical phenomena involved in propellant constituent packing, and their modeling via the ATK/Thiokol ParPack code. Dr. Davis and Dr. Beckstead plan to meet in the near future to continue work on this task. Responsibility for this task has been assigned to Dr. Davis of ATK/Thiokol.

D.3.2 Task 2. Combustion Models

The basic objective of this work is to couple the ATK/Thiokol ParPack code with BYU combustion codes to develop greater capability to predict solid propellant burning rates and agglomeration tendencies.

D.3.2.1 Task 2.1. Propellant Burnback Model

Responsibility for this task has been assigned to Dr. Beckstead of BYU.

The BDP model¹ from the 70s was based on a single, statistically average particle size for each AP fraction in a propellant. Thus, the geometric considerations were very simplified, but it did employ a very realistic, three flame, flame structure. The 1-D model considered the three separate flame zones and treated their interaction with simple global kinetics. Burning rate calculations for Miller's 21 non-aluminized propellants² were all within $\sim\pm10\text{-}15\%$ of the experimental data, with the exception of one formulation. The model also correctly predicted the effects of particle size and oxidizer concentration on burning rate.

Condon, Glick and Osborne^{3,4} extended the BDP concept by considering a more rigorous statistical description of the packing with their Petite Ensemble Model (PEM). Their results were slightly better than the BDP results. However, it is not clear if that was due to a more correct physical description, or due to the extra degrees of freedom from the additional parameters in their model.

Other models evolved, but none showed significantly improved accuracy, nor significantly improved physical interpretations (see Cohen's review paper⁵).

More recently, the development of codes to describe the geometrical packing of a solid propellant have evolved with the CSAR project at the University of Illinois^{6,7} and at ATK/Thiokol on the ParPack code.⁸ These models represent significant progress toward developing a realistic geometrical packing description of a solid propellant.

¹ M.W. Beckstead. Combustion calculations for composite solid propellants. *Proceedings of the 13th JANNAF Combustion Meeting*, Volume 2, pages 299–312. The Chemical Propulsion Information Agency, Applied Physics Laboratory, Johns Hopkins University, Laurel, MD. 1976.

² R.R. Miller, et al. Control of solids distribution in HTPB propellants. AFRPL-TR-78-14, 1978.

³ J.A. Condon and J.R. Osborn. The effect of oxidizer particle size distribution on the steady and nonsteady combustion of composite propellants. AFRPL-TR-78-17, 1978.

⁴ J.A. Condon and R. L. Glick. Statistical combustion modeling —The effect of additives. *Proceedings of the 14th JANNAF Combustion Meeting*, pages 341–378. The Chemical Propulsion Information Agency, Applied Physics Laboratory, Johns Hopkins University, Laurel, MD. 1977.

⁵ N.S. Cohen. Review of composite propellant burn rate modeling. *AIAA Journal* **18**(3):277–293, 1980.

⁶ L. Massa, et al. Three-dimensional heterogeneous propellant combustion. *Proceedings of the Combustion Institute* 29:2975–2983, 2002.

⁷ T.L. Jackson and J. Buckmaster. Heterogeneous propellant combustion. *AIAA Journal* 40(6):1122–1130, 2002.

⁸ I.L. Davis and R.G. Carter. Random particle packing by reduced dimension algorithms. *Journal of Applied Physics* 67(2):1022–1029, 1990.

However, combining the packing codes with a realistic flame model to calculate actual propellant burning rates is still a challenge. Preliminary results by CSAR are encouraging, but computational time, and the chosen kinetics model limit their progress.⁹ Their combustion model assumes the three flame BDP model, but with extremely simplified kinetics and diffusion. Their validation calculations have been limited to just four propellant formulations, three of which were within $\sim\pm 20\text{-}30\%$ of the data, but the fourth was worse. Considering the fact that there are eleven constants in their kinetic model, and they treat them as arbitrary constants, their validation is not impressive. Their model needs more validation calculations before any judgment can be made.

Figure D-1 shows the results of recent work at BYU incorporating realistic kinetics into a detailed numerical diffusion model which shows encouraging promise towards simulating the minute detail involved in determining the burning rates of AP containing propellants.¹⁰ These results show that the key factor in determining propellant burning rate is the primary diffusion flame reaction occurring between the AP and binder $\sim 10\text{-}20\ \mu\text{m}$ above the surface. To capture the actual physics, these reactions have to be modeled with appropriate chemistry and physics on a very small scale. To calculate a surface burning rate based on tens of particles on a surface, such as in the CSAR model, would require such a tiny grid that it would be cost prohibitive. Another approach must be considered.

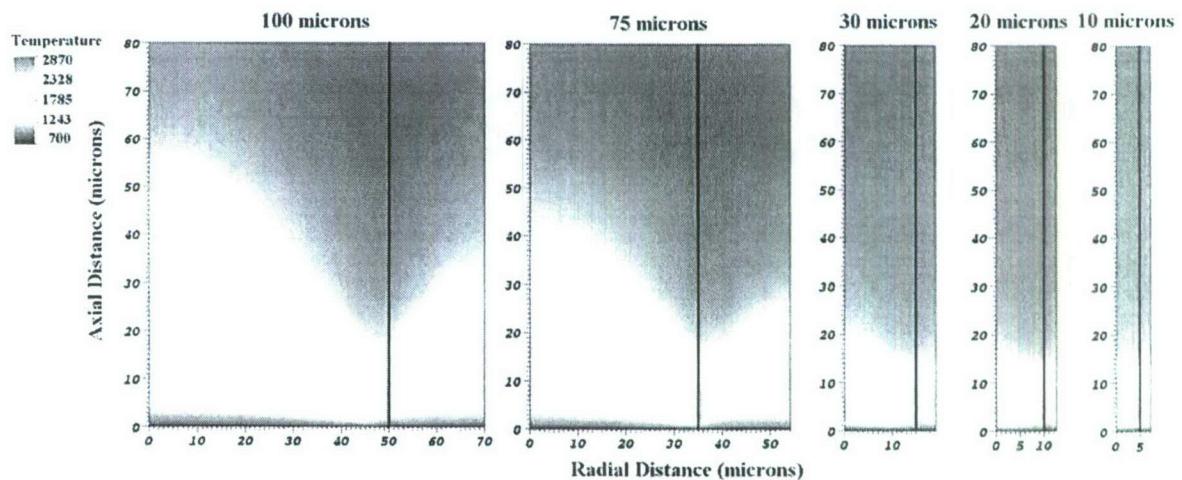


Figure D-1: Particle size effects on near-surface combustion

Based on the success of the BDP and PEM models, using simplified geometries, it is felt that a similar approach would be justified. It appears that a reasonably correct description of the diffusion flame is probably more important than a detailed description of the surface packing. Therefore, we are currently exploring the potential for coupling a series of time-resolved diffusion flame calculations for a single particle while varying its geometry from its initial state

⁹ L. Massa, T.L. Jackson and J. Buckmaster. New kinetics for a model of heterogeneous propellant combustion. *Journal of Propulsion and Power* 21(5): 914–924, 2005.

¹⁰ M.L. Gross, S. A. Felt and M. W. Beckstead. Two-dimensional modeling of AP composite propellants with detailed kinetics: Effects of particle size and pressure. AIAA-2006-4925, 2006.

through final burnout. This would give us a burning rate for that particle. Then, we would have to extract configurations for different sized particles from the ParPack code with an appropriate distribution of binder per particle. Summing these would allow us to simulate a burning propellant surface. Initial calculations will be made for Miller's non-aluminized propellant data set. ParPack calculations to generate packs of these formulations are currently underway.

Eventually, this effort will focus on evaluating the geometrical effects of particle size distributions on burning rate. The diffusion flame code will be run as a sub-grid model, varying pertinent parameters to develop correlations that can be coupled into the main code. The validation data will come from Miller's non-aluminized data set.² Then, for Task 2.2, Miller's aluminized propellant formulations² will be used for the agglomeration calculations.

D.3.2.2 Task 2.2. Surface Agglomeration Model

Responsibility for this task has been assigned to Dr. Hylin of SEA and Dr. Beckstead of BYU.

SEA has done a number of statistical calculations on surface agglomeration data collected by ATK/Thiokol using quench-bomb tests and the Microtrac® particle measuring system.¹¹ That data had been reported as part of the IHPRT effort. No very clear trends emerged from the statistics. However the statistics do suggest a significant link between the agglomerate diameter and the initial diameter of the aluminum particles (or some function thereof). The other significant correlation was with burning rate. Paradoxically, the statistics also seem to support Dr. Beckstead's observation that the agglomerate diameter does not correlate with burning rate at constant pressure, but neither is there a significant correlation with pressure when the effects of pressure are separated from the effects of propellant formulation.

Given that the experimental data identify some significant factors but no clear trends, it seems likely that the most reliable approach to predicting surface agglomeration should combine the salient experimental factors with a model based on chemico-physical principles. A detailed examination of window bomb movies and quench bomb data seems to indicate that ignition of an agglomerate appears to be the dominant mechanism in determining the agglomerate size. The agglomeration task will therefore focus on using ParPack to calculate separation distances for the various AP crystals in a formulation. These calculations will then be loosely coupled to the diffusion flame calculations to determine ignition sources on the surface.

Different definitions of separation distance will be explored to determine a viable algorithm. Eventually, the agglomeration task will develop a definitive ignition/separation distance algorithm for coupling into the main code. Validation data will come from parallel programs utilizing rotating quench bomb results for ATK/Thiokol propellants, and from high resolution window bomb movies from China Lake.

Work on this task is in a preliminary state. BYU personnel will be working closely with ATK/Thiokol personnel to help overcome practicality problems. The BYU work will utilize the ATK/Thiokol ParPack code, but will recognize and maintain the proprietary aspects of the code.

¹¹ Leeds & Northrup Co, St. Petersburg, Florida 33702. Microtrac®.

D.3.2.3 Task 2.3. Al Burning Rate Model Selection

Responsibility for this task has been assigned to Dr. Hylin of SEA and Dr. Beckstead of BYU. As previously reported, we are reviewing the analytical burn rate models of King¹², Turns¹³, and Law¹⁴, as well as the empirical models of HermSEN¹⁵ and Beckstead.¹⁶

D.3.3 Task 3. Review and Select Droplet Models

Responsibility for this task has been assigned to Dr. Hylin of SEA and Dr. Eaton of ATK/Thiokol.

D.3.3.1 Droplet Drag Model

As a droplet leaves the burning grain surface and thereafter, its ballistic trajectory is directed by aerodynamic drag. The ballistic calculation therefore must incorporate a suitable drag model. Since we are dealing with an accelerating compressible flow, models which are functions of the relative droplet Mach number as well as the droplet Reynolds number are to be preferred over a simple Reynolds number dependence.

The modified Crowe model used in SPP¹⁷ is a good baseline against which other candidate models may be judged. It is described by the following equations:

$$C_D = (C_{D_0} - 2)e^{-3.07\sqrt{\frac{M}{Re}}g(Re)} + \frac{h(M)}{\sqrt{\gamma}M}e^{-Re/2M} + 2, \quad (D-1)$$

$$g(Re) = \frac{1 + Re(12.278 + 0.584 Re)}{1 + 11.278 Re} \quad \text{for } Re \leq 10^3, \quad (D-2)$$

$$h(M) = \frac{5.6}{M + 1} + 1.7\sqrt{\frac{T_p}{T}}, \quad (D-3)$$

$$C_{D_0} = \begin{cases} 24 / Re & \text{for } 0 < Re \leq 0.34 \\ 0.48 + 28 Re^{-0.85} & \text{for } 0.34 < Re \leq 10^5 \end{cases} \quad (D-4)$$

Hylin¹⁸ has developed a formula for C_{D_0} that yields a slight improvement in the fit to the original ($M = 0$) data, especially at Reynolds numbers above 100:

¹² M. King. Aluminum droplet combustion. Contract report for Software and Engineering Associates, Inc. 2006.

¹³ S. R. Turns, S. C. Wong and E. Ryba. Combustion of aluminum-based slurry agglomerates. *Combustion Science and Technology*, 54, 1987.

¹⁴ C. K. Law and F. A. Williams. On a class of models for droplet combustion. AIAA-74-147, January 1974.

¹⁵ R. W. HermSEN. Aluminum combustion efficiency in solid rocket motors. AIAA-81-0038, January 1981.

¹⁶ K. P. Brooks and M. W. Beckstead. Dynamics of aluminum combustion. *Journal of Propulsion and Power*, 11(4):769-780, 1995.

¹⁷ G.R. Nickerson, et al, A computer program for the prediction of solid propellant rocket motor performance (SPP).AFRPL-TR-83-036, Volume 1, 1984.

¹⁸ E. C. Hylin. Working notes on the drag law for spheres. Unpublished, 19 January 2004.

$$C_{D_0} = \frac{24}{\text{Re}} \left(1 + \frac{3}{16} \text{Re} \right) \left(\frac{1 + 0.0059 \text{Re}}{1 + 0.065 \text{Re}} \right) \quad \text{for } 0 < \text{Re} \leq 10^5. \quad (\text{D-5})$$

The first factor in this formula is due to Stokes, the second to Oseen, and the third to Hylin.

According to the SPP Final Report, the modified Crowe model described above contains simplifications that limit its range of applicability to $\text{Re} < 10^3$ and reduce its accuracy when $M > 2$. These restrictions were not considered a limitation in SPP, since the maximum likely value of Re was regarded as being generally less than 50, and the maximum likely value of the droplet relative Mach number M was regarded as being generally less than 2. In GTBL simulations, however, we have observed values of Re as high as 700. Apparently, the simplifications adopted by SPP were made for the sake of reducing the computer memory and run-time required for the droplet drag calculations in TD2P. With the vast improvement in computers that has taken place since then, memory and run-time are no longer issues in that respect, and the simplifications should perhaps be revisited in the interest of having a model that is more generally applicable.

D.3.3.2 Droplet Agglomeration Model

The droplet agglomeration model was described in the previous progress report. On further review, however, it was determined that the expression for the Stokes number as given by Salita¹⁹ was not correct. The velocity difference used in calculating the Stokes number should in this case be that between the two colliding particles, not that between the gas and the larger particle. Thus we should have

$$\text{St} = \left(\frac{2}{9} \right) \frac{\rho_{mp} |\mathbf{V}_s - \mathbf{V}_L| R_s^2}{\mu_{gas} R_L}, \quad (\text{D-6})$$

With the velocity difference given by

$$|\mathbf{V}_s - \mathbf{V}_L| = \sqrt{(\mathbf{V}_s - \mathbf{V}_L) \cdot (\mathbf{V}_s - \mathbf{V}_L)}. \quad (\text{D-7})$$

Calculations using our selected agglomeration model have been made using SEA's GTBL code. The change in how the Stokes number was calculated was shown to have negligible effect for the cases considered.

Figure D-2 shows the growth in radius for agglomerating droplets in an Extended Delta motor, as predicted by GTBL using the agglomeration model we have described. Three droplet groups were used in this calculation, with initial radii of 1.5, 2.8 and 10.3 μm . The figure shows droplet radii for the largest group, which are seen to increase in the downstream direction as collision and coalescence take place. The increase is most rapid in the regions where differential aerodynamic drag forces have pulled the large and small droplets onto intersecting paths.

¹⁹ M. Salita. Implementation and validation of the one-dimensional gas/particle flow code OD3P. *Proceedings of the 26th JANNAF Combustion Meeting*, Volume 2, pages 69–81. The Chemical Propulsion Information Agency, Applied Physics Laboratory, Johns Hopkins University, Laurel, MD. 1989.

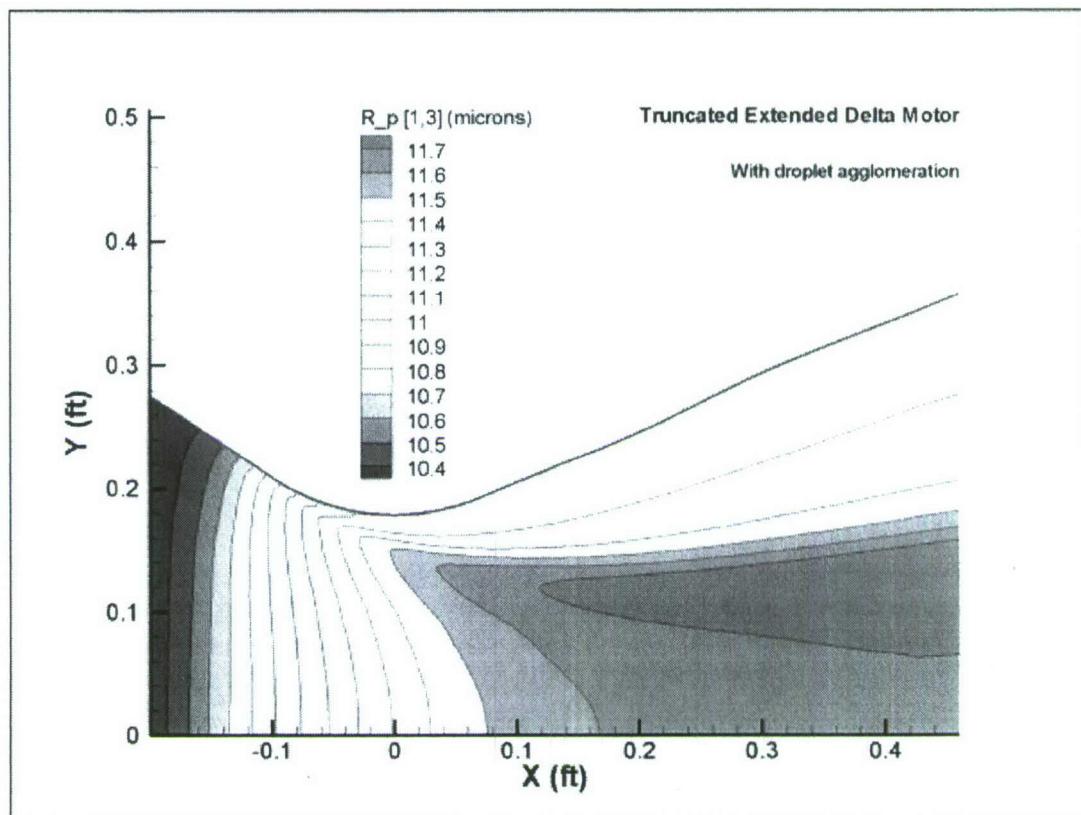


Figure D-2: Radius field contours for agglomerating droplets

Meanwhile, Figure D-3 shows the mass flowrates for the three droplet groups, and how these rates change as the droplets collide and coalesce with each other. The figure shows an increase in the mass flowrate of the largest droplets at the expense of the smallest, as the latter collide with and are absorbed by the former. The middle group also participates in collisions, but for this group the effects of collisions with the smaller and larger particles nearly offset.

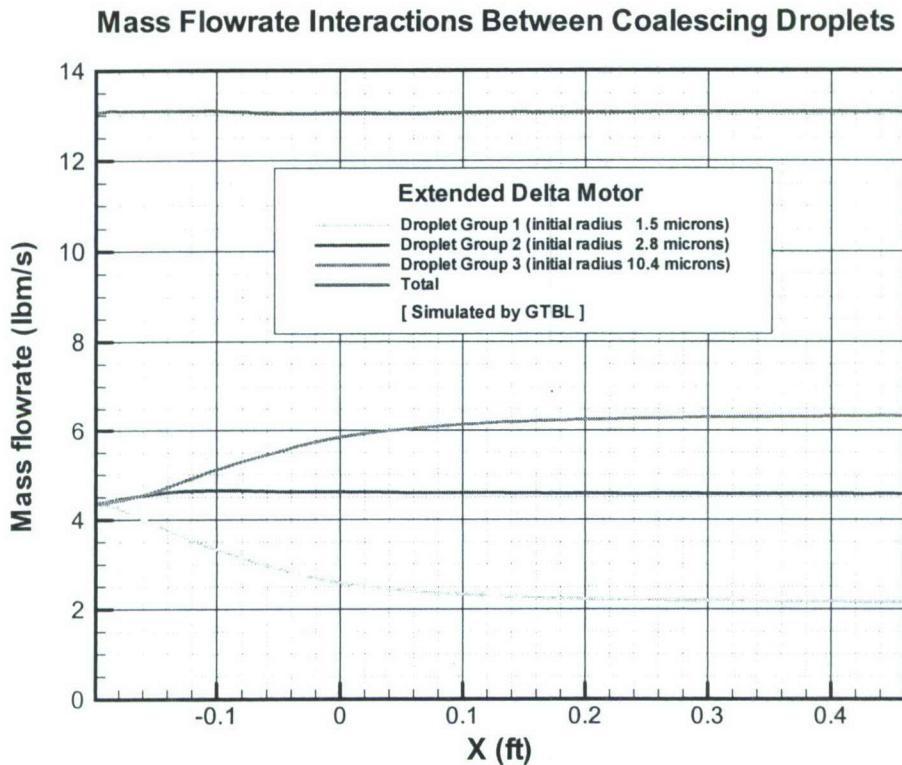


Figure D-3: Mass flowrates for agglomerating droplets

D.3.3.3 Droplet Breakup Models

We previously reported that we were considering two alternative models for droplet fragmentation: 1) a critical Weber-number criterion; and 2) Taylor Analogy Breakup (TAB)²⁰. Since then we have determined that there are two variants on the Weber-number criterion; these are not always explicitly distinguished in the literature, and they exhibit somewhat different behavior.

One of the Weber-number criteria, which we shall designate the *pure* Weber-number criterion, specifies that droplet fragmentation occurs when

$$\frac{2R\rho_{\text{gas}} |\mathbf{V}_p - \mathbf{V}_g|^2}{\sigma} > \text{We}_{\text{crit}}, \quad (\text{D-8})$$

in which R is the droplet radius, ρ_{gas} is the gas-phase density, $|\mathbf{V}_p - \mathbf{V}_g|$ is the magnitude of the difference between the droplet and gas-phase velocities, σ is the surface tension of the droplet, and We_{crit} is some critical value.

²⁰ P. J. O'Rourke and A. A. Amundsen. The TAB method for numerical calculation of spray droplet breakup. Los Alamos National Lab, NM. National Technical Information Service publication DE87011756, 1987.

The original criterion from Bartlett and Delaney²¹, however, may be expressed as

$$\frac{2R\rho_{\text{gas}}|\mathbf{V}_p - \mathbf{V}_g|^2}{\sigma} > \frac{8}{C_D}, \quad (\text{D-9})$$

in which C_D is the coefficient of drag. Now if we express the drag coefficient in terms of the Stokes drag, with a proportionality coefficient of C_D^\dagger , that is:

$$C_D = \frac{24}{\text{Re}} C_D^\dagger, \quad (\text{D-10})$$

then the Bartlett and Delaney criterion becomes

$$\frac{2R\rho_{\text{gas}}|\mathbf{V}_p - \mathbf{V}_g|^2}{\sigma} > \frac{1}{3} \frac{\text{Re}}{C_D^\dagger}. \quad (\text{D-11})$$

Noting that the droplet Reynolds number

$$\text{Re} = \frac{2R\rho_{\text{gas}}|\mathbf{V}_p - \mathbf{V}_g|}{\mu_{\text{gas}}}, \quad (\text{D-12})$$

the Bartlett and Delaney criterion simplifies to

$$\text{Ca} = \frac{|\mathbf{V}_p - \mathbf{V}_g| \mu_{\text{gas}}}{\sigma} > \frac{1}{3C_D^\dagger}. \quad (\text{D-13})$$

The left-hand side of this expression takes the form of a Capillary-number, which does not depend on the droplet radius. Meanwhile the right-hand side depends only weakly on the radius through the Reynolds-number dependence of C_D^\dagger .

In both the model using the pure Weber-number criterion — Inequality (D-8) — and the model using the Bartlett and Delaney Capillary-number criterion — Inequality (D-13) — droplet fragmentation is supposed to occur instantaneously when the criterion is satisfied, with the original droplet breaking up into n smaller droplets of equal size. The difference in action between the two models is that after fragmentation, the new, smaller droplets are likely to be far from satisfying Inequality (D-8), but quite close to satisfying Inequality (D-13) a second time. We will use SEA's IHPPT M&S-developed combustion efficiency code CEFR to investigate the practical differences between these two models.

Aerojet, as part of their IHPPT work²², has investigated the TAB model. In attempting to simulate an experiment of Craig, they found that the quality of the simulation results depended on the proper selection of the TAB model constants. With appropriate values for the constants, they were able to get a good match between the simulation results and the experimental data, as illustrated in Figure D-4.

²¹ R.W. Bartlett and L.J. Delaney. Effect of liquid surface tension on maximum particle size in two-phase nozzle flow. *Pyrodynamics*, 4:337–341, 1966.

²² Aerojet-General Corporation, Sacramento, California, IHPPT solid rocket motor modeling and simulation program, IPT-9 presentations, Contract No. F04611-03-C-0041.6–7 September 2006.

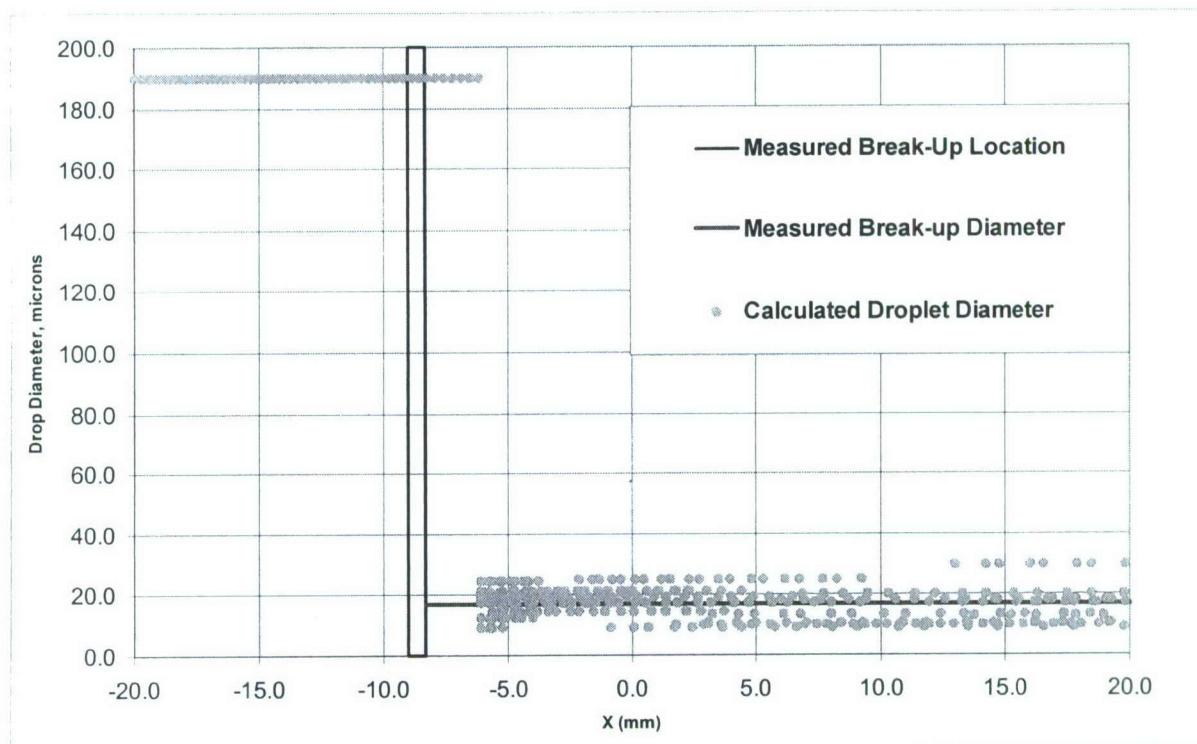


Figure D-4: Aerojet simulation²² of particle breakup — Craig experiment; Initial droplet size of 190 μm .

Proper selection of the model constants, the critical Weber-number We_{crit} in particular, is also necessary when using the Weber-number criterion for breakup. As originally formulated, the Bartlett and Delaney model, whether in the form of Inequality (D-9) or the form of Inequality (D-13), does not have an explicit control constant for the fragmentation threshold. We can introduce one as a factor on the right-hand side of the inequality. Denoting this factor by C_{crit} , Inequality then becomes

$$\text{Ca} = \frac{|\mathbf{V}_p - \mathbf{V}_g| \mu_{\text{gas}}}{\sigma} > \frac{C_{\text{crit}}}{3C_D^{\dagger}}. \quad (\text{D-14})$$

Near the end of their paper, Bartlett and Delaney mention that Lane's experiments with water droplets²³ suggest a value of 0.5 for C_{crit} . In general, however, we should expect that We_{crit} , C_{crit} , or the TAB model constants might need to be recalibrated for different problems.

Model example calculations using Equation (D-8) have been made using SEA's GTBL code. Figure D-5 shows the results of these calculations for three droplet groups, plotted along a typical gas streamline in an Extended Delta motor. For these calculations it was assumed that $\text{We}_{\text{crit}} = 5.90$, and that on fragmentation each drop would split into $n = 8$ smaller drops of equal size. The initial droplet radii were 27 μm , 50 μm , and 93 μm . As seen in the figure, the final radii for all three groups were around 5 μm .

²³ W. R. Lane. *Ind. Eng. Chem.*, 43:1313–1317, 1951. Cited in Bartlett and Delaney²¹.

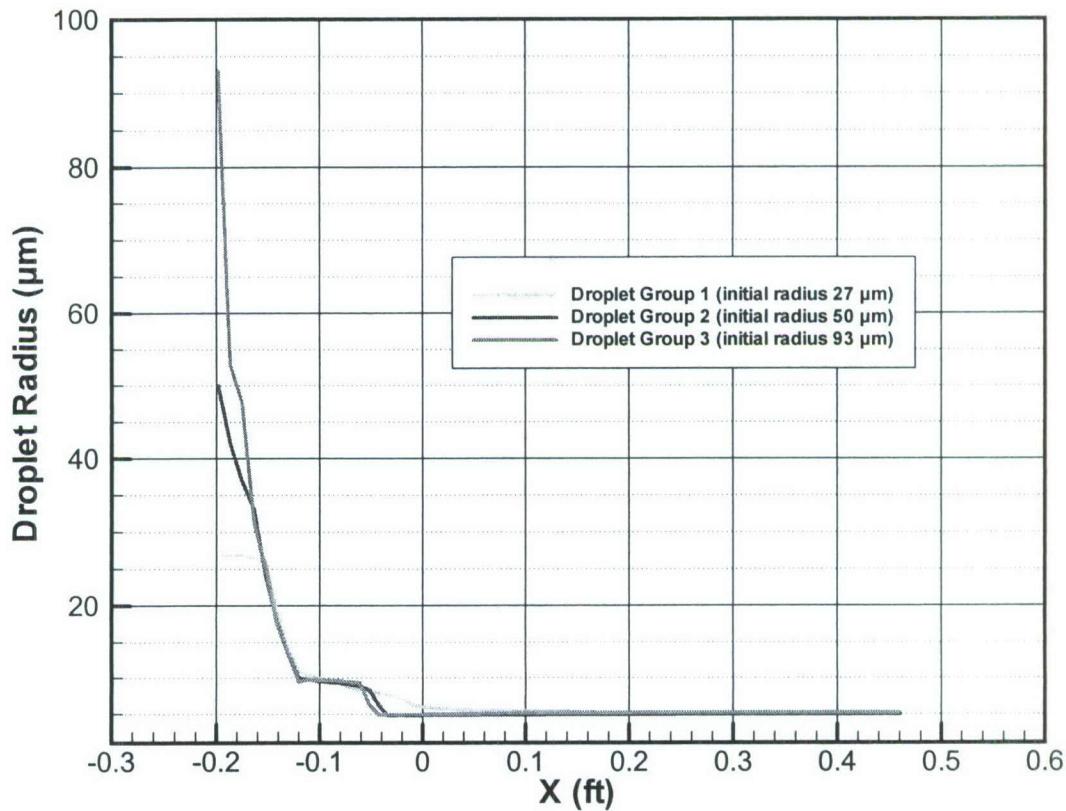


Figure D-5: Droplet fragmentation as calculated by Weber-number model, along a typical gas streamline in an Extended Delta motor

On the basis of the above results, it appears that either a Weber-number criterion or the TAB approach should be adequate for modeling droplet fragmentation. At present there does not seem to be any strong reason for preferring one over the other. Consequently, we would consider implementing both, if that is feasible, and leave the choice of model up to the user.

D.3.4 Task 4. Review and Select Models of Droplet Impact, Erosion, and Heat Transfer

Responsibility for this task has been assigned to Dr. Eaton of ATK/Thiokol and Dr. Hylin of SEA.

D.3.4.1 Droplet Impact and Erosion

Work has not yet begun on the review and selection of models for droplet impact and associated erosive effects, although the HERO2D^{24,25} particle impact and erosion model developed by ATK/Thiokol under the IHPPT program is a likely candidate.

D.3.4.2 Droplet Heat Transfer

ATK/Thiokol have developed a droplet impingement heat transfer code²⁶ for the IHPPT program. We will have access to this as part of the IHPPT modeling effort. (ATK/Thiokol are also under subcontract to us on the present contract). Results from some preliminary calculations using this code were reported by Ewing, et al²⁷, and are shown in the following figures.

Figure D-6 shows the predicted nozzle surface temperatures at several positions, under the influence of heat transfer from impinging droplets of molten alumina. The temperature curves are clearly seen to break down into the three time-periods predicted by Hylin, Coats and Dunn.^{28,29} As described by those authors, these time periods are

1. The *early or fast transient* period, during which the wall surface temperature is less than the melting temperature of alumina. During this period impinging droplets freeze to the wall, yielding their latent heat and building up a layer of solid alumina on the surface.
2. The *intermediate or transition* period. This period sees the melting of the solid alumina layer that was built up during the fast transient, and the absorption of latent heat during the melting process serves to maintain the wall temperature at approximately the alumina melting temperature.
3. The *late or slow transient* period, during which the wall temperature is at or above the melting temperature of alumina. During this period the continued mass flux of impinging droplets contributes to the presence of a layer of liquid alumina on the surface of the nozzle wall, while the forces from the flowing gas continue to convect this liquid downstream. Eventually this layer becomes very thin.

²⁴ M. E. Ewing, D. T. Walker and D. A. Isaac. Development of a two-dimensional numerical code for modeling pyrolysis and ablation. To be presented at the *JANNAF 54th JPM, 3rd LPS, 2nd SPS, and 5th MSS Joint Meeting*, Denver, CO, 14-17 May 2007.

²⁵ D. A. Isaac, D. T. Walker and M. E. Ewing. Description of the two-dimensional heat transfer and erosion analysis code — Hero2D. To be presented at the *JANNAF 54th JPM, 3rd LPS, 2nd SPS, and 5th MSS Joint Meeting*, Denver, CO, 14-17 May 2007.

²⁶ M. E. Ewing and P. H. Bauer. Numerical modeling of accretion and heat transfer in rocket nozzles due to condensed-phase impact. To be presented at the *JANNAF 54th JPM, 3rd LPS, 2nd SPS, and 5th MSS Joint Meeting*, Denver, CO, 14-17 May 2007.

²⁷ M. E. Ewing, et al, *SRM Modeling Development Program, IPT Meeting #10, ATK Thermal Model Development* (Presentation). Contract No. F04611-03-C-0043, CDRL Data Item A003. ATK 7 February 2007.

²⁸ E. C. Hylin, D. E. Coats, and S. S. Dunn. Alumina impingement literature review and analysis. AFRL-PR-ED-TR-2003-0038, November 2003.

²⁹ E.C. Hylin, D.E. Coats, and S.S. Dunn. Modeling nozzle heat transfer from alumina impact. *Proceedings of the 39th JANNAF Combustion Meeting* The Chemical Propulsion Information Agency, Johns Hopkins University, Columbia, MD. 2003.

Ewing, et al.²⁷ refer to these three time-periods as the *rime regime*, the *glaze regime*, and the *liquid-only regime*, referring to the state of the slag accumulation on the nozzle wall.

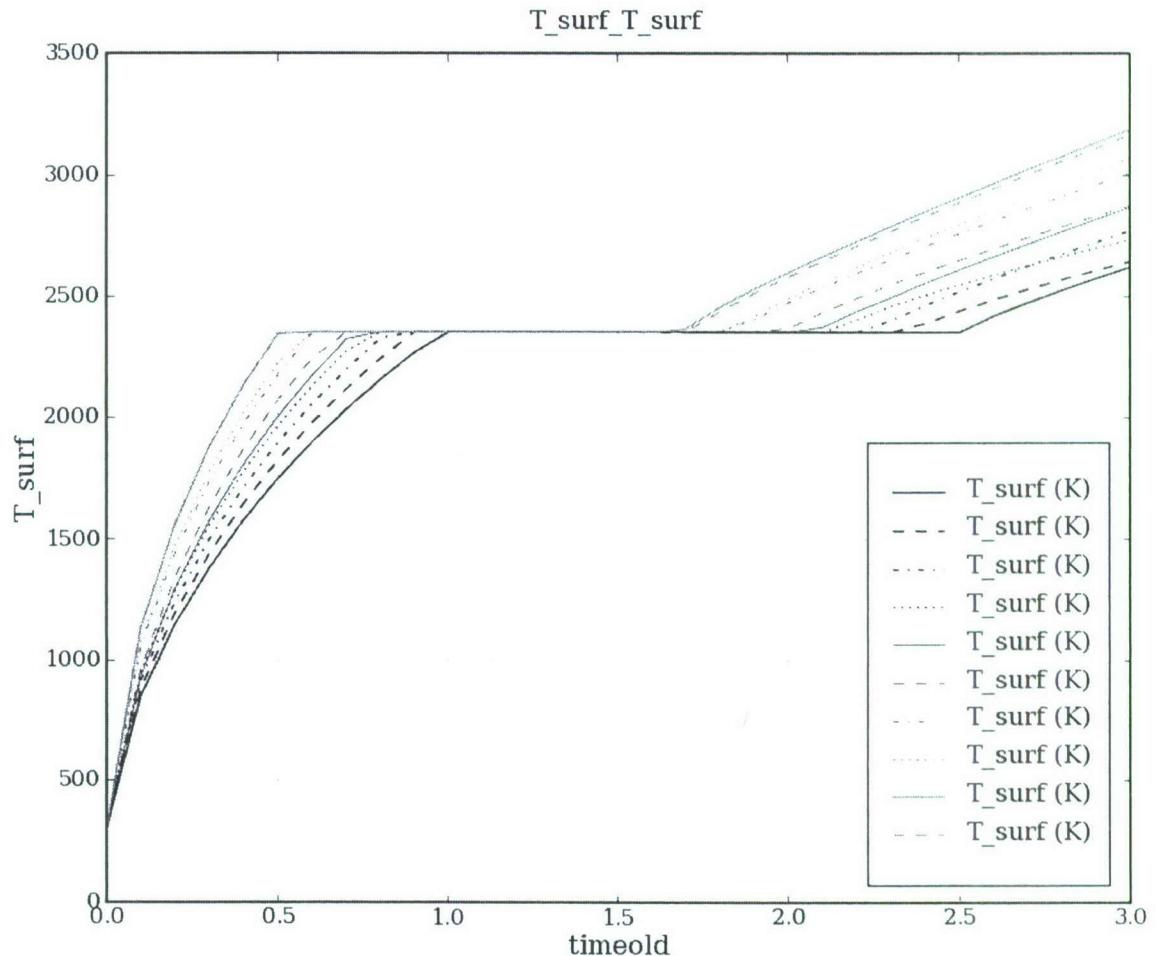


Figure D-6: Predicted²⁷ nozzle surface temperatures under droplet impingement

Figure D-7 shows the predictions made by Ewing, et al.²⁷ for the slag thickness on the nozzle surface. At each location along the wall, the initial linear rise in the slag-layer thickness is followed by a break in the curve at the point where the surface of the slag begins to melt. This break corresponds to the division between the rime regime and the glaze regime. As the slag melts it is convected downstream and the thickness of the layer gradually decreases to almost nothing, in accordance with the prediction of Hylin, Coats and Dunn.^{28,29}

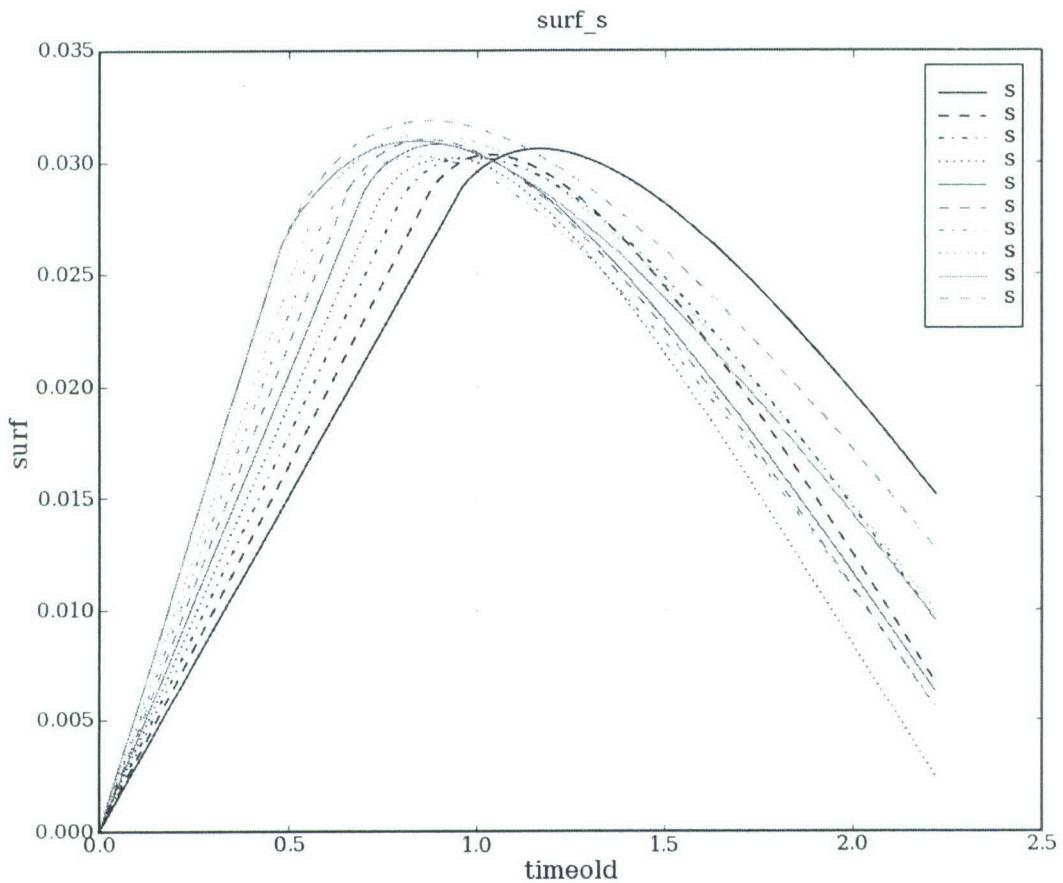


Figure D-7: Predicted²⁷ nozzle surface slag thickness under droplet impingement

Figure D-8 shows the interfacial heat fluxes predicted by Ewing, et al. Again, the different phenomena occurring during the three time-periods are reflected in the shape of the heat flux curves.

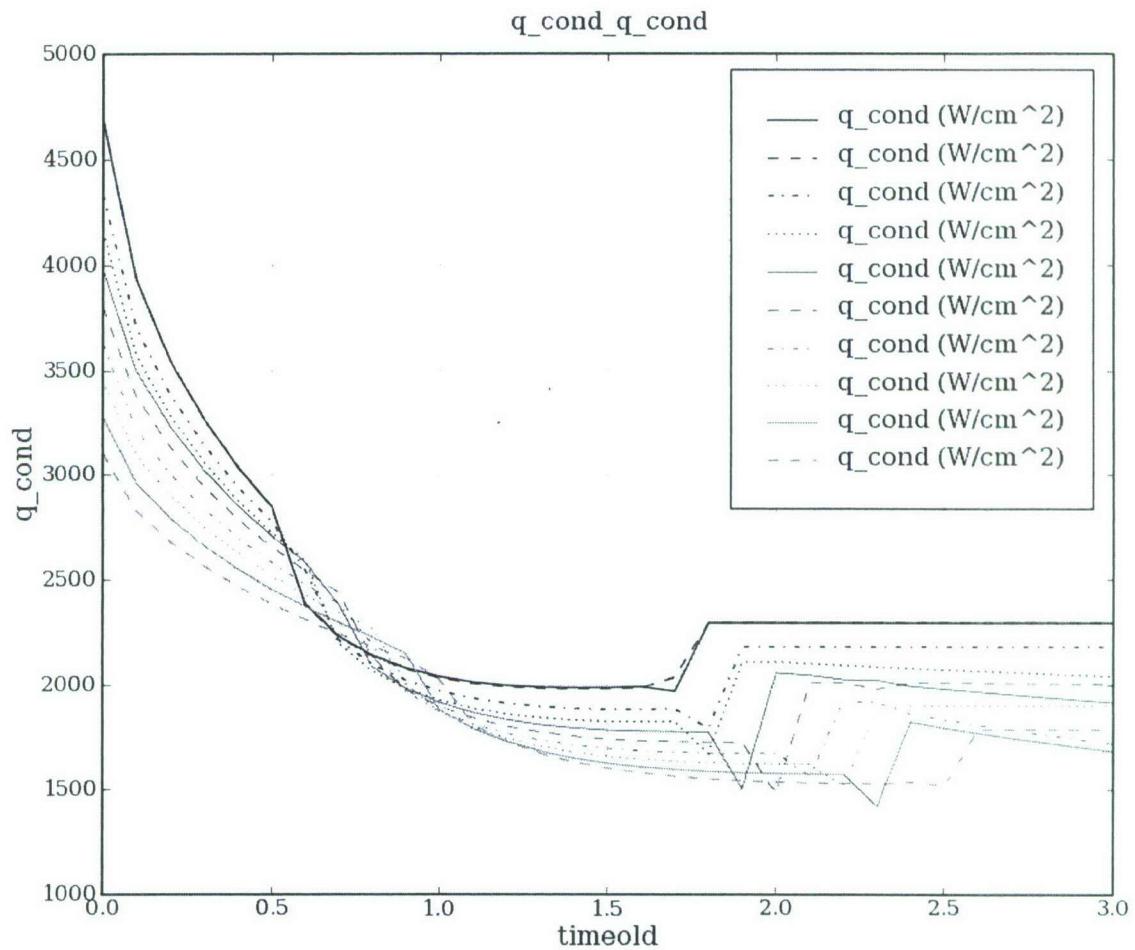


Figure D-8: Predicted²⁷ nozzle interface heat flux under droplet impingement

D.3.4.3 Thermochemical Erosion

Our review of thermochemical ablation models has begun by considering the work done to date by SEA on insulation and nozzle erosion as part of the IHPPT M & S effort. In that work, a step by step procedure was established to evaluate the thermo chemical response of a hypothetical graphitic throat insert to a ASRM thermal environment. This calculation involves 3 program modules: 1) the TD2P module, which calculates inviscid Boundary Layer edge conditions, 2) the CCET module, which calculates the gas/wall chemistry and ablation potential, and 3) MACE, which calculates the thermo chemical response. Special provision was made to distinguish the carbon originating from the wall material from the carbon originating from the propellant. Salient results of this calculation for the ablation potential and for the surface recession rate are shown in Figure D-9 and Figure D-10.

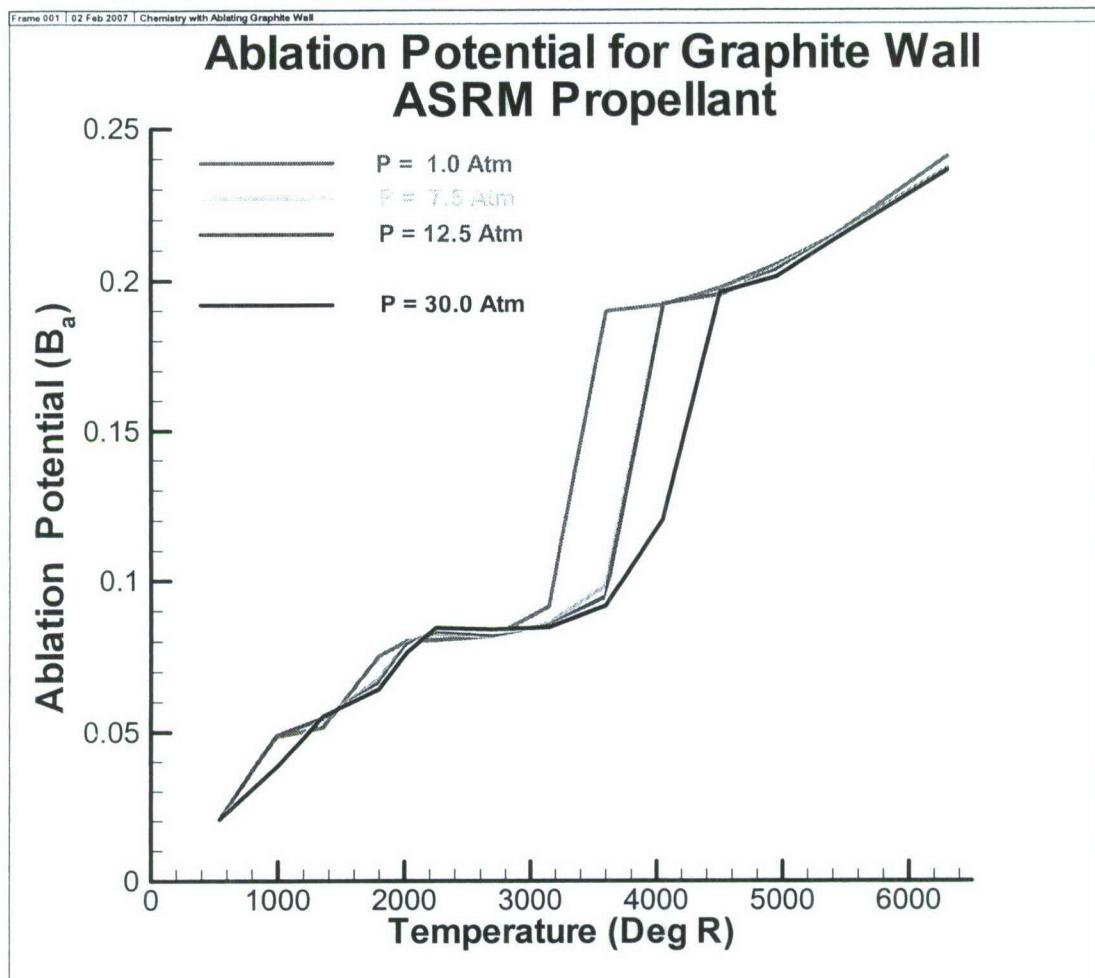


Figure D-9: Ablation potential for graphite wall, ASRM propellant

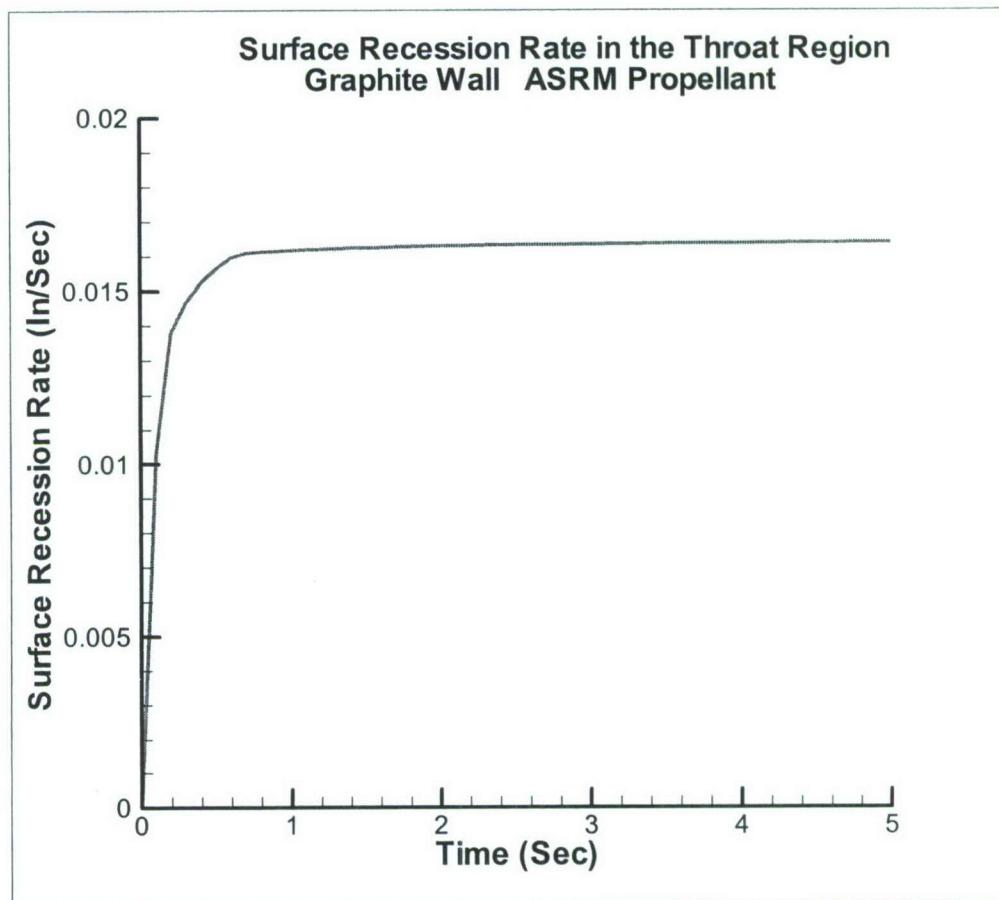


Figure D-10: Surface recession rate in the throat region

The thermochemical erosion model incorporated in this analysis was originally developed for re-entry vehicle thermal protection systems in the 1960's. This model was subsequently adapted for rocket propulsion systems with a similar degree of success. Although there are many assumptions and simplifications made in this model, a multitude of test data has validated this approach and methodology.

Since the development of this model, computing power has greatly increased, potentially allowing relaxation of the above simplifications. Unfortunately, even with the introduction of massively parallel computing systems, the computing power required to model this problem in full theoretical detail is still prohibitive — instead of taking minutes, a typical higher order analysis would take months. In addition, the uncertainty associated with many of the sub-models (such as the turbulence model) and non-validated input variables (such as the coefficients associated with the kinetic/catalytic gas wall reaction rates) suggest that a theoretically more precise or detailed solution would not be justified at this time.

D.3.5 Task 5. Review and Select Computer Framework

Responsibility for this task has been assigned to Dr. Hylin of SEA and Dr. Eaton of ATK/Thiokol.

Initially, SEA's SPP code and ATK/Thiokol's FEM-BUILDER code were considered as candidate frameworks for the aluminum combustion and flow solver models. Concurrent work performed by SEA as part of the IHPRT program is producing a Perl³⁰-based driver script for SPP and other codes. This script calls each module as an individual executable. Communications between modules will be coordinated by this script through various data files. At present, this script exists only in command line mode, though a graphical interface is being planned for future development.

The main goal of the new SPP design is to allow a user to select which module will analyze each portion of the motor. For example, a user could choose between running the FCT, ATA, or GTBL modules for the transonic analysis, and then pass the results of the selected module to a nozzle module for the next step. This design approach will also ease maintenance and improve the capability for upgrades to SPP.

Positioning a high-level driver script on top of SPP and/or FEM-BUILDER and other codes appears to offer a very general and flexible framework. Such a framework is likely to facilitate the integration and inter-operation of aluminum-combustion and flow-solution modules within SPP, and between SPP and other codes. It also facilitates the development and perhaps even the automatic configuration of a graphical user interface via the GTK+ toolkit³¹ and gtk2-perl³².

Perl is a stable, cross-platform programming language. It is very well-suited to manipulating text-based files, such as the input and output files used by SPP. This makes it an ideal scripting language for the task at hand. GTK+ is a multi-platform toolkit for creating graphical user interfaces. It is free software, developed as part of the GNU Project. It is licensed under the GNU LGPL, which allows it to be used by all developers, including those developing proprietary software, without any license fees or royalties. Gtk2-perl is the collective name for a set of perl bindings for GTK+ and various related libraries. These modules make it easy to write graphical applications using Perl.

Development of a graphical user interface built on the GTK+ toolkit can be further facilitated by a rapid-design tool called Glade³³. The user interfaces designed in Glade are saved as XML³⁴ files, and by using the *libglade* library these can be loaded by applications dynamically as needed. Since these interface definitions are written in XML, they can also be prepared by hand, or by the transformation of other XML files. This offers the possibility of at least partially automating the generation of graphical user interface elements for the driver script, if the input and output data interfaces for SPP and other supported codes can themselves be described in

³⁰ The Perl directory. <http://www.perl.org/>, 2007.

³¹ GTK+ — The GIMP toolkit. <http://www.gtk.org/>, 2007.

³² Gtk2-perl. <http://gtk2-perl.sourceforge.net/>, 2007.

³³ Glade User Interface Builder. <http://glade.gnome.org/>, 2007.

³⁴ I. S. Graham and L. Quin. *XML Specification Guide*. John Wiley & Sons, 1999.

XML. Nothing precludes this in principle, but a suitable Document Type Definition (DTD) must be evolved. The level of effort that would be required is appropriate to Phase II. We also plan to compare the approach in which SPP and its modules are driven by a Perl-script to the approach taken by FEM-BUILDER. If these approaches are complementary, they can even be integrated. SEA is exploring the possibility of licensing the FEM-BUILDER code from ATK/Thiokol.

D.4 Management and Cost

D.4.1 Progress

Except as noted above in Sections 0 and 0, the contract is on schedule and we are reviewing our program plan to make sure that all elements of it are on track.

D.4.2 Management

There were no management issues during this reporting period.

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APPENDIX E: BYU FINAL REPORT

**Modeling Solid Propellant
Combustion and Agglomeration
Using the ATK ParPack Code**

Final Report

In support of STTR Contract: FA 9550-06-C-0069
Through
SEA, Carson City, Nevada

Submitted by
Merrill W Beckstead
Brigham Young University

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Task Objective:

The basic objective of this work is to couple the ATK/Thiokol ParPack code with BYU combustion codes to develop greater capability to predict solid propellant burning rates and agglomeration tendencies

Task 1: Coupling an Effective Combustion Code with ParPack

The BDP model¹ from the 70s has provided the basis for understanding the mechanisms determining propellant combustion for over three decades. It was based on a single, statistically average particle size for each AP fraction in a propellant. Thus, the geometric considerations were very simplified, but it did employ a very realistic, three flame, flame structure. The model correctly predicted the effects of particle size and oxidizer concentration on burning rate for typical composite propellants.

More recently, the development of codes to describe the geometrical packing of a solid propellant have evolved with the CSAR project at the University of Illinois^{2,3} and at ATK/Thiokol on the ParPack code.⁴ These models represent significant progress toward developing a realistic geometrical packing description of a solid propellant.

However, combining the packing codes with a realistic flame model to calculate actual propellant burning rates is still a challenge. Preliminary results by CSAR are encouraging, but computational time and the chosen kinetics model limit their progress.⁵ Their validation calculations have been very limited.

Figure E-1 shows the results of recent work at BYU incorporating realistic kinetics into a detailed numerical diffusion model shows encouraging promise towards simulating the minute detail involved in determining the burning rates of AP containing propellants.⁶ These results show that the key factor in determining propellant burning rate is the primary diffusion flame reaction occurring between the AP and binder \sim 10-20 μm above the surface. To capture the actual physics, these reactions have to be modeled with appropriate chemistry and physics on a very small scale. To calculate a surface burning rate based on tens of particles on a surface, such as in the CSAR model, would require such a tiny grid that it would be cost prohibitive. Another approach must be considered.

¹ Beckstead, M. W., "Combustion Calculations for Composite Solid Propellants," 13th JANNAF Combustion Meeting, 1976, CPIA #281, Vol. 2, pp 299-312.

² Massa, L., Jackson, T.L., Buckmaster, J. and Campbell, M., " Three-dimensional Heterogeneous Propellant Combustion", Proc. of the Combustion Institute, 2002, 29, pp. 2975-2983.

³ Jackson, T.L. and Buckmaster, J., " Heterogeneous Propellant Combustion," AIAA J, Vol. 40, No. 6, pp. 1122-1130.

⁴ Davis, I. L. and Carter, R. G., "Random Particle Packing by Reduced Dimension Algorithms," *Journal of Applied Physics*, Vol. 67, No. 2, 1990, pp. 1022-1029.

⁵ Massa, L., Jackson, T.L. and Buckmaster, J., " New Kinetics for a Model of Heterogeneous Propellant Combustion," *J. Prop. and Power*, Vol. 21, No. 5, 2005, pp. 914-924.

⁶ Gross, M. L. Felt S. A. and Beckstead M. W. Two-Dimensional Modeling of AP Compositie Propellants with Detailed Kinetics: Effects of Particle Size and Pressure. AIAA-2006-4925. 2006.

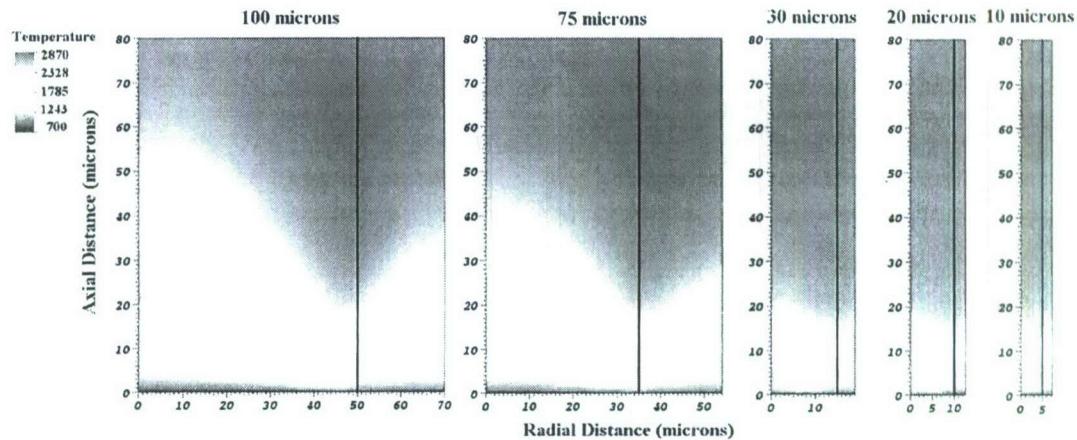


Figure E-1. Temperature profiles for three particle diameters: a) 400 μm , b) 100 μm and c) 75 μm . 77.5% AP in binder, 0.86 overall AP mass fraction, P=20atm.

Based on the success of the early BDP model, using a simplified geometry, it is felt that a similar approach is justified. It appears that a reasonably correct description of the diffusion flame is probably more important than a detailed description of the surface packing. Therefore, we are currently exploring the potential for coupling a series of time resolved diffusion flame calculations for a single particle, but varying its geometry from its initial state through final burnout. This would give us a burning rate for that particle. Then, we would have to extract configurations for different sized particles from the ParPack code with an appropriate distribution of binder per particle. Summing these would allow us to simulate a burning propellant surface.

In order to accomplish this, an accurate model of the diffusion flame is needed. The result of Figure E-1 are very encouraging, but were made for a single geometry. Additional calculations are required varying the geometry. As the geometry varies the oxidizer/fuel ratio will also vary. Thus, a kinetic model is required that allows a significant variation in the AP/HTPB concentrations. The kinetic model used to make the calculations in Figure 1 was based on the Jeppson AP/HTPB mechanism⁷ that was developed to model homogenized binder formulations varying the AP concentration from 75% to 80%.

More recently a generalized kinetic mechanism has been developed to model a variety of ingredients, including nitramines, azides and nitrate esters. The details of this effort are summarized in a review paper by Beckstead, et. al.⁸ The original Jeppson AP/HTPB mechanism was developed independent of the work involving other ingredients. For the current effort, it was felt that an AP/HTPB mechanism should be compatible with the generalized mechanism, if calculations were to be made for aluminized propellants having lower concentrations of AP, e.g.

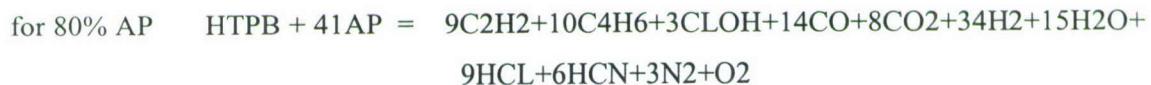
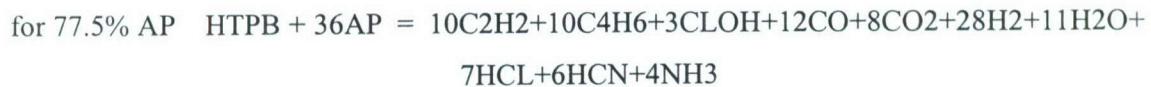
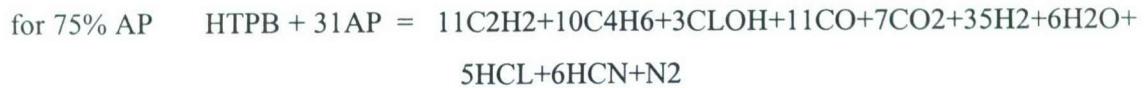
⁷ Jeppson, M. B., Beckstead, M. W. and Jing, Q., *A Kinetic Model for the Premixed Combustion of a Fine AP/HTPB Composite Propellant*, 36th Aerospace Sciences Meeting & Exhibit, AIAA-98-0447, (1998).

⁸ Beckstead, M.W., Puduppakkam, K.V., Thakre, P. and Yang, V., "Modeling of Combustion and Ignition of Solid Propellant Ingredients," *Progress in Energy and Combustion Science*, 2007, (in press).

~ 70% AP. Thus, the second half of the BYU SSTR effort was focused on developing a more compatible AP/HTPB kinetic mechanism.

Initially, combining the generalized mechanism with the Jeppson AP/HTPB mechanism produced unsatisfactory results. Apparently the generalized mechanism produced too many alternate kinetic pathways for the AP and HTPB combustion species, resulting in an unrealistically low predicted burning rate. Recent work by Gross, et.al.⁹ developing a compatible AP mechanism, was first incorporated into the generalized mechanism. Then, a modified AP/HTPB condensed phase mechanism was developed to determine the surface species required for the surface boundary condition to the modified, generalized mechanism.

The modified AP/HTPB condensed phase mechanism that has been developed is:



These three global reaction mechanisms give the consistent AP to HTPB ratio from 75 to 80% by varying the amount of AP entering the reaction. The product species are typical of those observed by Korobeinichev¹⁰ and by Brill.¹¹ Their data are not entirely consistent with each other, and thus only provide qualitative information about the surface species. The requirements for the calculations are to predict within reason: 1) the burning rate, 2) the adiabatic flame temperature, 3) the major equilibrium species, and 4) a consistent trend for the surface species as they vary with AP concentration.

Calculations were performed using the modified AP/HTPB mechanism, simulating propellants with varying AP percentage for 75, 77.5 and 80 percent, all at 20 atm. Figure E-2 shows the comparison between the calculated and measured data of Foster¹² for his 12 μm AP monomodal propellant. The agreement is excellent.

⁹ Gross, M. L., Felt S. A. and Beckstead M.W., "Two-Dimensional Modeling of AP Composite Propellants with Detailed Kinetics: Effects of Particle Size and Pressure," AIAA-2006-4925. 2006

¹⁰ Korobeinichev, O. P., et al., *Flame Structure, Kinetics and Mechanism of Chemical Reactions in Flames of Mixed Composition Based on Ammonium Perchlorate and Polybutadiene Rubber*, Combustion, Explosion & Shock Waves, Vol. 28, No. 4, pp. 53-59, (1992).

¹¹ Brill, T.B., P.E. Gongwer, and B. Budenz, "Condensed-Phase Oxidizer-Binder Chemistry During Flash Pyrolysis," *34th JANNAF Combustion Meeting*, (1997), Vol. II, CPIA #662, pp. 447-456.

¹² Foster, R.L. and R.R. Miller, "The Burn Rate Temperature Sensitivity of Aluminized and Non-Aluminized HTPB Propellants," *1980 JANNAF Propulsion Meeting*, (1981), CPIA #315, Vol. IV, pp. 667-693.

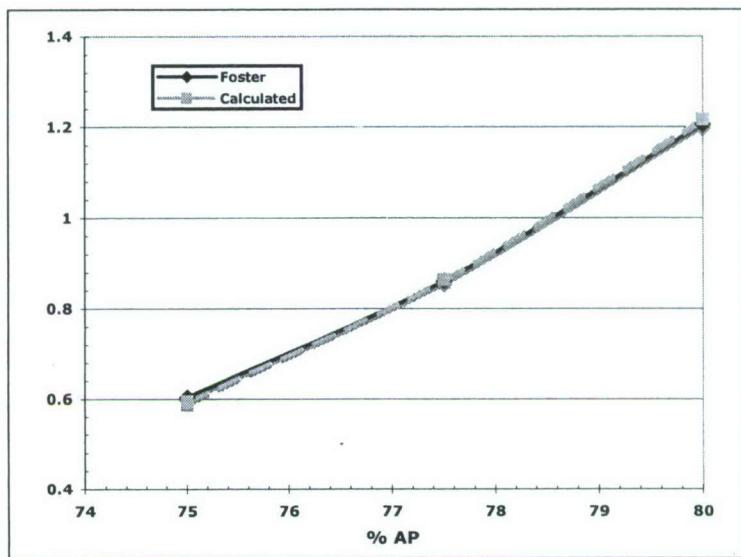


Figure E-2. Comparison of calculated and measured burning rates for 75% AP, 77.5% AP and 80% AP at 20atm.

Figure E-3 shows the comparison between the calculated and equilibrium flame temperatures.

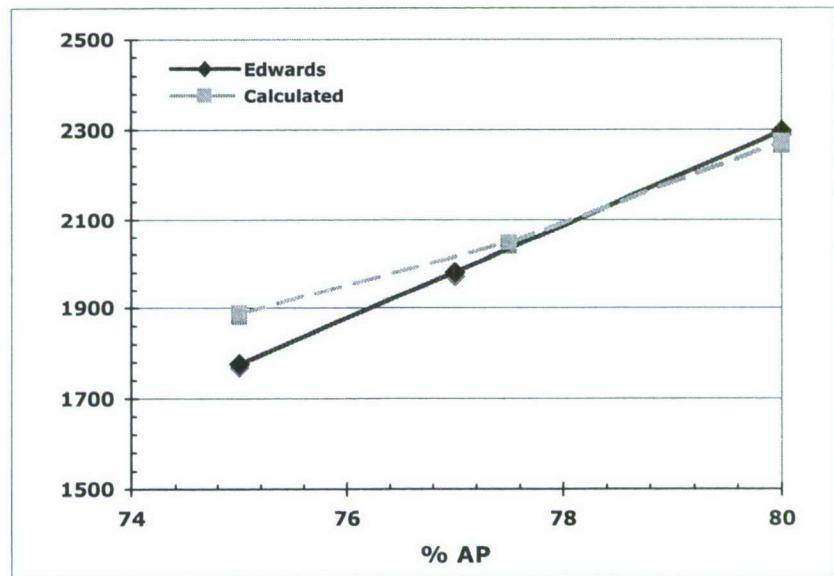


Figure E-3. Comparison of calculated and equilibrium temperatures for 75% AP, 77.5% AP and 80% AP at 20atm.

Figure E-4 shows the comparison between the calculated and equilibrium species concentrations.

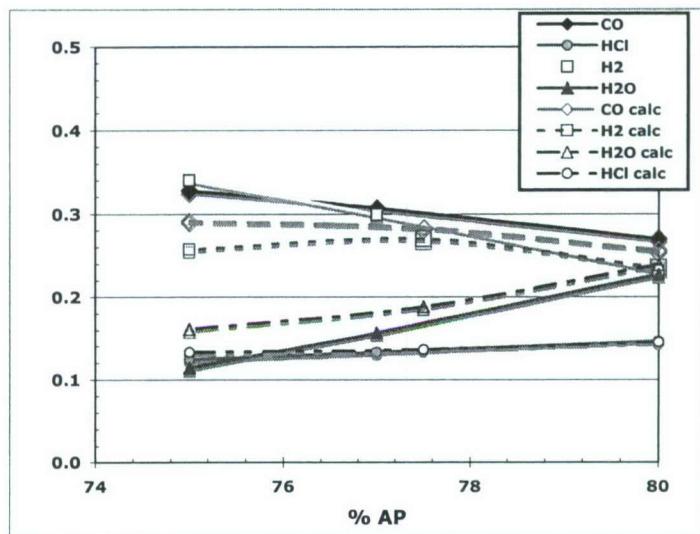


Figure E-4. Comparison of calculated and equilibrium species for 75% AP, 77.5% AP and 80% AP at 20atm.

Figure E-5 shows the calculated surface species for the three formulations. Although there are not any quantitative data to compare to, the predicted trends with varying AP percentage appear to be self consistent.

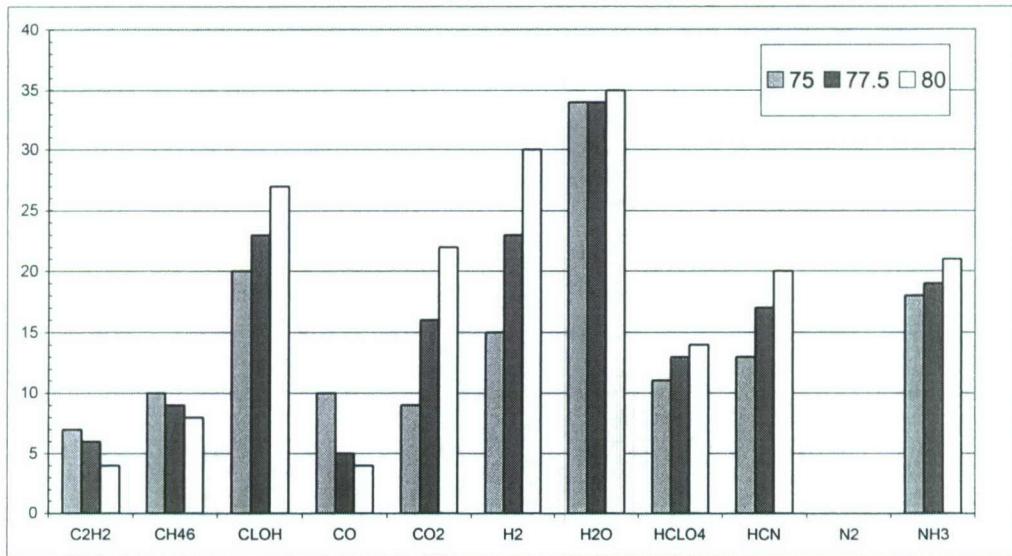


Figure E-5. Comparison of calculated surface species for 75% AP, 77.5% AP and 80% AP at 20atm.

The calculations indicate that the proposed AP/HTPB mechanism appears to be consistent with the available data and equilibrium temperature and species products. Thus, this mechanism will be able to be used for diffusion flame calculations for propellant geometries that give distributions in this range.

Task 2: Developing a Consistent Agglomeration Model Using ParPack

The agglomeration task was to focus on using ParPack to calculate separation distances for the various AP crystals in a formulation. These calculations would then be loosely coupled to the diffusion flame calculations to determine ignition sources on the surface. A detailed examination of window bomb movies, and quench bomb data seems to indicate that ignition of an agglomerate appears to be the dominant mechanism in determining the agglomerate size.

This task was intended to be undertaken as part of the Phase II contract, which has not been funded.

Summary and Conclusions

The primary contribution of the second half of the STTR contract was the development of an AP/HTPB mechanism that is compatible with the generalized BYU kinetic mechanism and that is consistent with the available data and equilibrium information for mixtures of AP and HTPB varying from 75 to 80% AP.

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APPENDIX F: ATK FINAL REPORT

Particle packing studies for Software Engineering Associates
Final Report*

Michael Webb and I. Lee Davis
Predictive Aging Team

Motor Health Management Department
ATK Launch Systems, Inc.

October 18, 2007

Summary

This report documents particle packing studies ATK Launch Systems performed to support Software Engineering Associates' study of aluminum agglomeration in Minuteman propellant combustion. The report begins with an overview of the modeling tool used, then presents the propellant data input to the model, and concludes with the modeling results.

Description of the ParPack particle packing tool

This section describes a Monte Carlo particle packing computer code called ParPack which can create particle packs consisting of spherical particles. The distinguishing feature of ParPack is that it employs a reduced dimension algorithm that permits the construction of packs with very broad particle size distributions. For a more detailed exposition of this tool, see the paper by Webb and Davis.¹²³

The key to this reduced-dimension approach is to represent each particle of a different size or density (*a mode*) in the pack by its own cylinder, scaled appropriately to the particle's size. We define a particle mode to be all particles in a pack that are indistinguishable relative to one or more properties of interest. A monomodal pack comprises a single cylinder (and is in fact equivalent to a three-dimensional pack). A binary pack includes two concentric cylinders, whose radii are scaled proportionally to the size of each particle. A ternary pack comprises three cylinders, and so on. All cylinders share a common axis, but the cylinder radii depend on each particle's size.

Methodology

We construct the pack by dropping particles at a randomly chosen position within each particle's cylinder. When simulating more than one particle mode, the order in which the particles are dropped is also random (respecting the final number of each particle mode required to represent the desired mass fraction of each mode). Each particle is dropped above the pack and allowed to descend into the pack under the influence of a unidirectional force field (e.g., gravity) acting along the *z*-axis until the particle finds a contact stability point. Until the particle finds a stability

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¹²³Random particle packing with large particle size variations using reduce-dimension algorithms, M. D. Webb and I. L. Davis, Pow. Tech. 167 (2006) 10-19.

point, it will roll along other particles or the roll corridor defined by one or more particles and/or the cylinder wall. Contact stability refers to whether the current sphere is in compressive contact with an object or in tensile contact. If it is in compressive contact with another sphere or the cylinder wall, the particles push against each other due to the current sphere's weight. When a particle touches three or more objects compressively, it is stable and is placed at that position. When in tensile contact with another particle or the cylinder wall, the current sphere will roll away from the object unless it already has three or more compressive contacts. After the particle is placed at a contact stability point, another particle is dropped and the sequence repeated until completion (all particles dropped and stable).

As we build the pack, each particle mode remains within its own cylinder. The smallest mode particle resides in the smallest cylinder, and is closest to the axis of symmetry. Larger particles may lie within the inner cylinders, but also extend into outer cylinders; each mode is always constrained to remain within its own cylinder. The largest particle in the pack may lodge in any of the cylinders, and in the outermost cylinder it resides alone. It should be clear that setting all cylinders to be the same size (the size of the largest particle's cylinder) produces a three-dimensional simulation. The implementation we have chosen thus allows us to build simulated packs with both reduced- and three-dimensional approaches by simply choosing each particle's cylinder size appropriately.

Advantage of the reduced-dimension approach

The development of the reduced-dimension approach to particle packing provides the opportunity to analyze particle packs with broad size distributions which would otherwise be computationally prohibitive. A full, three-dimensional simulation of 600,000 particles in a ternary pack with size ratios of 30:50:175 consumes 40 hours (real-time) on a fast desktop PC, placing approximately four particles per second. A reduced-dimension simulation which produces comparable statistical results runs in two minutes, placing 170 particles per second. This computational advantage increases tremendously as the particle size ratio increases. We recently investigated a composite material consisting of four particles of varying sizes with a maximum size ratio of 77:1; the reduced-dimension simulation modeled $3 \cdot 10^6$ particles and required about 100 hours to complete. We estimate that a three-dimensional simulation of the same fidelity would have required about $15 \cdot 10^9$ particles and about 100 years computer time with our simulation.

In general, we find that for equal numbers of particles, the algorithm's time to completion as a function of the particle size ratio R varies as $R^{3.3}$ for a fully three-dimensional simulation, but only as $R^{0.4}$ using the reduced dimension algorithms. Using the reduced-dimension approach, the algorithm time to completion as a function of the number of particles N is linear in N , with a particle size ratio of about 7-10:1. In three dimensions, the same calculation varies as N^3 . The reduced-dimension algorithm brings the simulation of complex particle packs with large particle size variation into the realm of possibility.

Detailed analysis of the simulation results, including the resulting pack structure, demonstrates conclusively that the reduced-dimension approach produces numerically identical results (within statistical uncertainty) to three-dimensional simulations, but at much less cost. In some cases, the reduced-dimension algorithm allows calculation of microstructure for packs that would otherwise be unattainable with existing methods.

In Figure F-1 we show a cross-section of a pack built with the ParPack tool. This pack was built using the reduced-dimension algorithm in ParPack, but in the figure we show only the innermost cylinder of the pack.

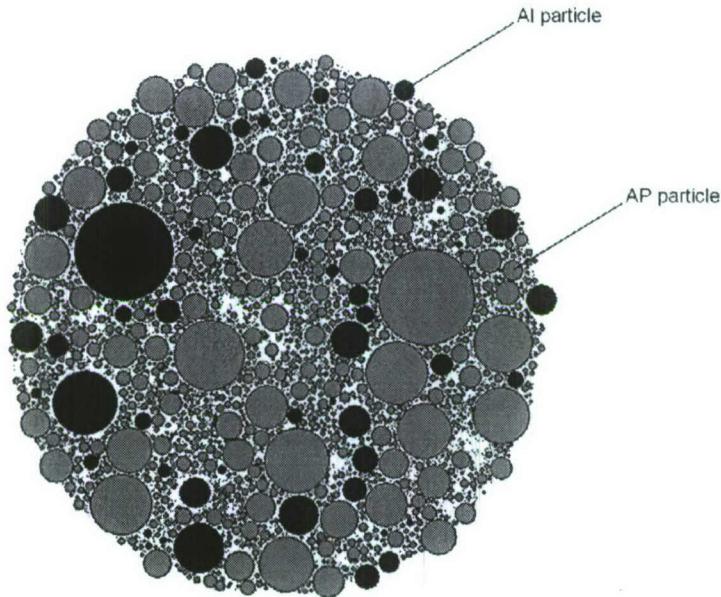


Figure F-1: Example particle pack showing Al (dark) and AP (light) particles for the Minuteman first-stage propellant mix analyzed in this study.

Minuteman propellant data

The packing studies performed for this project incorporated the “standard” Minuteman first-stage propellant recipe. This recipe comprises 70% ammonium perchlorate (AP), 16% aluminum, 12.18% PBAN polymer, and 1.82% epoxy curing agent. Typically, the AP distribution comprises particles of three different sizes (which are themselves distributed, not monomodal): 20 microns, 200 microns, and 400 microns. The relative ratio of the contributions of these particles in the propellant mix has varied over time. In the studies reported here, we used nominal values of 8.5% 400-micron AP, 31.5% 200-micron AP, and 30% 19-micron AP. Figure F-2 illustrates the total AP and Al distributions used in this study.

Study results

SEA requested that we provide to them statistics on the variation of the total AP perimeter and area at a given cross-section as a function of height in a particle pack. They desire to use this information in the development of their combustion and agglomeration tools.

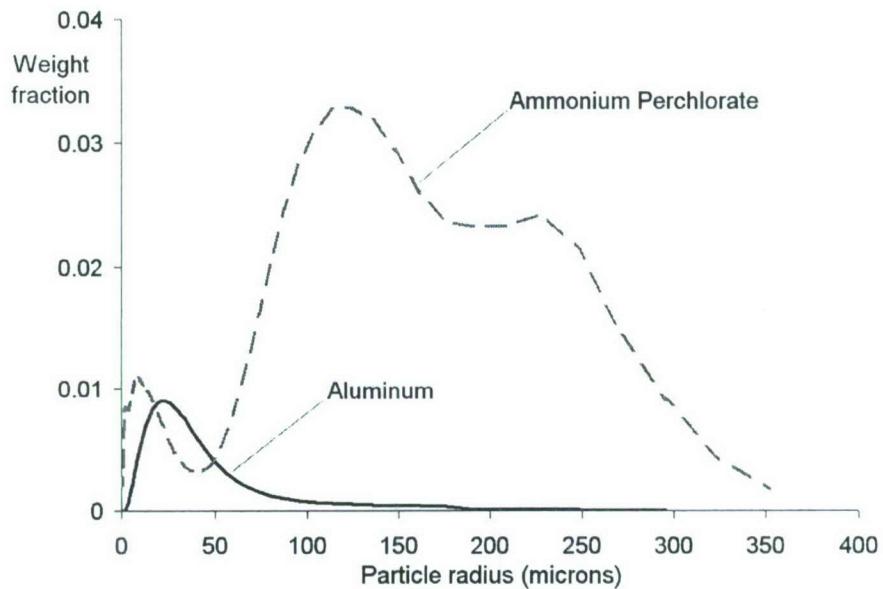


Figure F-2: Distribution of particle sizes for Al (line) and AP (dashed) used in the particle packing studies reported in this paper. The AP distribution is a composite of the different AP particle sizes used in the propellant mix.

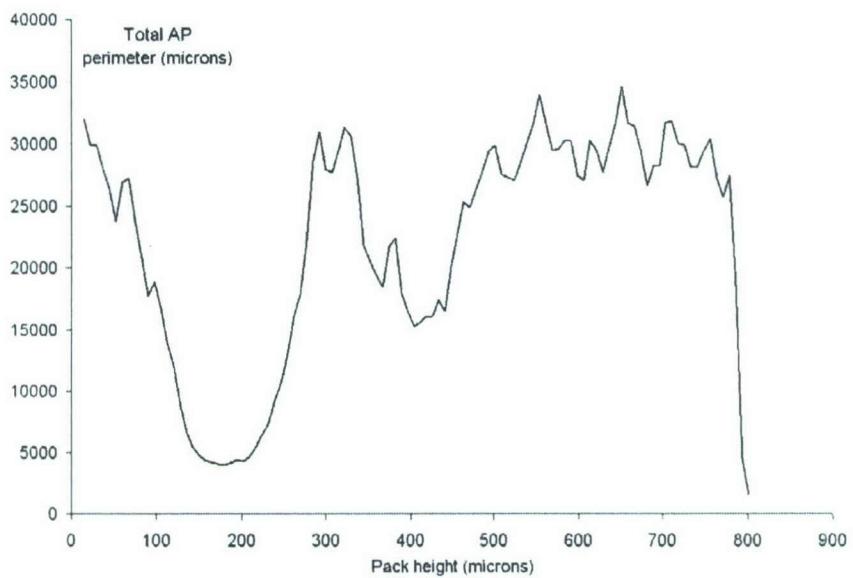


Figure F-3: This figure shows the total AP perimeter as a function of height in the particle pack. The large dip near a height of 200 microns is due to two large AP particles which nearly filled the innermost cylinder at that height during growth. A similar, though less pronounced peak occurs near a height of 400 microns.

We used the previously discussed propellant composition data to build two separate particle packs of about 1,000,000 particles each. The innermost cylinder of these packs had a diameter of 300 microns (per SEA request), and the total height of the packs was about 1 mm.

We analyzed the built packs as a function of height in the pack to determine the total local area and perimeter obtained by the AP particles. In Figure F-3, we show the total perimeter obtained by the AP particles as a function of height in the pack. The data shows a pronounced dip in the AP perimeter near a height of 200 microns in the pack. This is caused by two large AP particle of diameter 230 microns which lodged in the central cylinder during pack growth. A similar dip occurs near a height of 400 microns where a single AP particle of diameter 176 microns lodged near the wall of the central cylinder.

In Figure F-4, we show the total area of the AP particles as a function of height. The total area of the AP particles does not demonstrate the dips found in the perimeter data (for the obvious reason that the large particles nearly fill the cylinder).

Finally, in Figure F-5 we show the total number of particles in a given cross-section of the pack as a function of pack height. A particle is in the cross-section if it lies within one radius of the height under consideration. This chart shows the type of variability seen in the pack constituents as the pack grows.

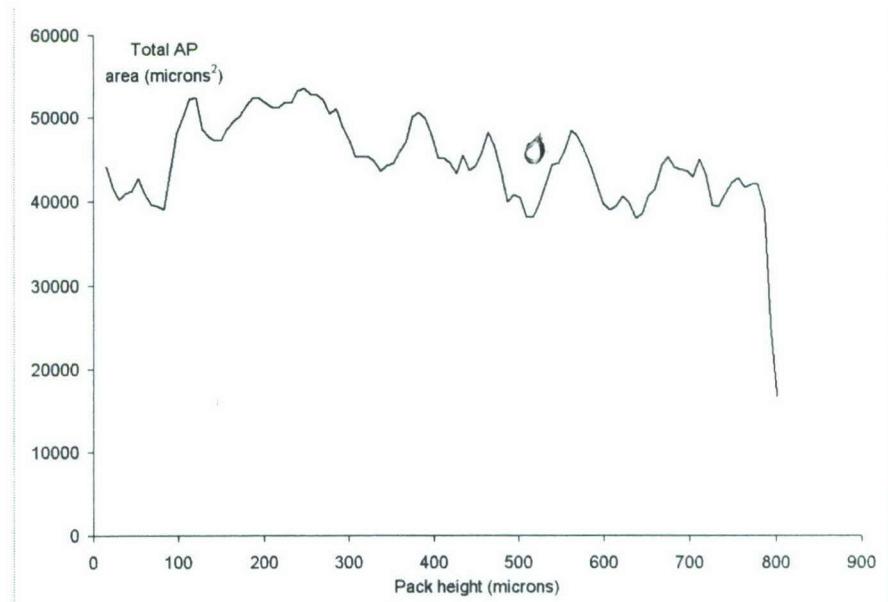


Figure F-4: This figure shows the total AP area as a function of height in the particle pack.

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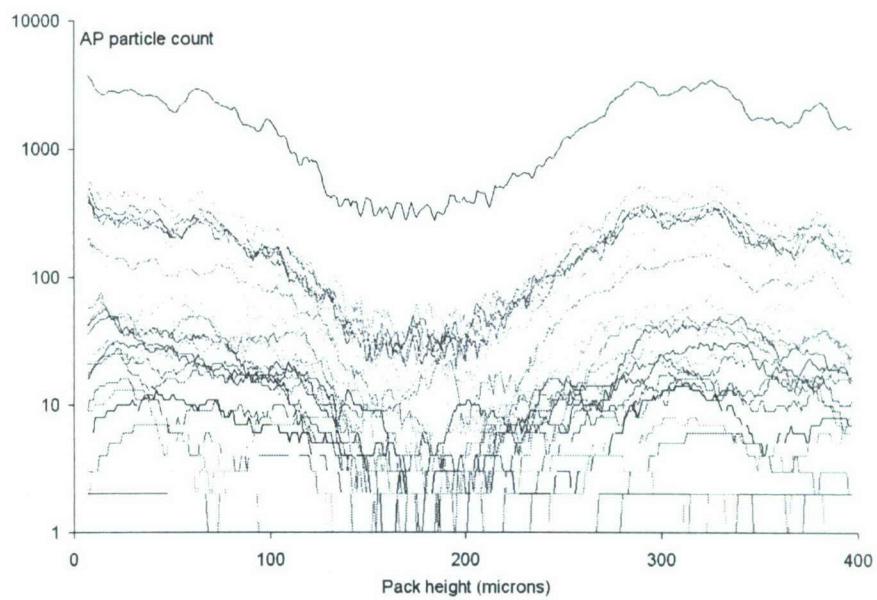


Figure F-5: This figure shows the number of AP particles of a given size in a given cross-section as a function of height in the particle pack. Note the logarithmic scale on the y-axis.

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